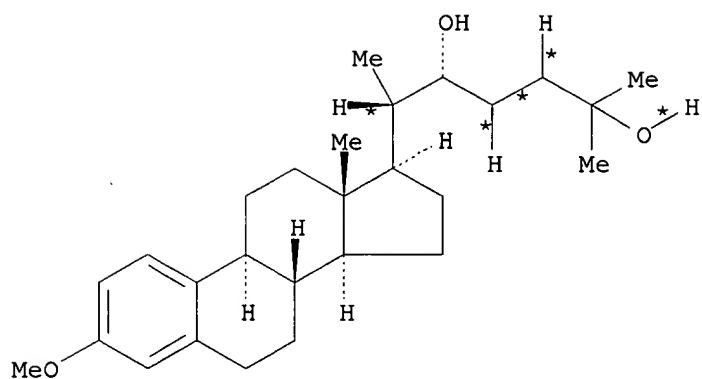


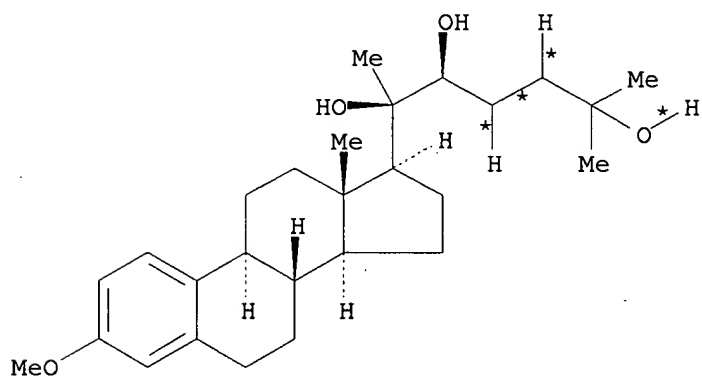
09/926,491

Page 1

=> d ibib ab hitstr 1-3



Z



AA

RX(9) RCT R **97452-84-1**, Q 97452-83-0

STAGE(1)

RGT U 7601-90-3 HClO₄

SOL 7732-18-5 Water, 67-56-1 MeOH

STAGE(2)

RGT V 1333-74-0 H₂

CAT 1314-15-4 PtO₂

PRO Z **97452-85-2**, AA 97452-86-3

L3 ANSWER 4 OF 4 CASREACT COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 103:71583 CASREACT

TITLE: A stereoselective synthesis of 1,2-diols from
.alpha.-hydroxyaldehydesAUTHOR(S): Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.;
Russell, Graeme B.; Horn, Dennis H. S.

CORPORATE SOURCE: Dep. Chem., Univ. Wyoming, Laramie, WY, 82071, USA

SOURCE: Tetrahedron Letters (1985), 26(9), 1189-92

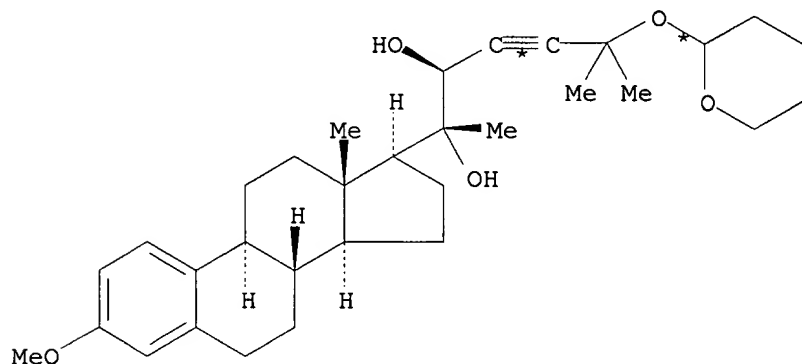
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

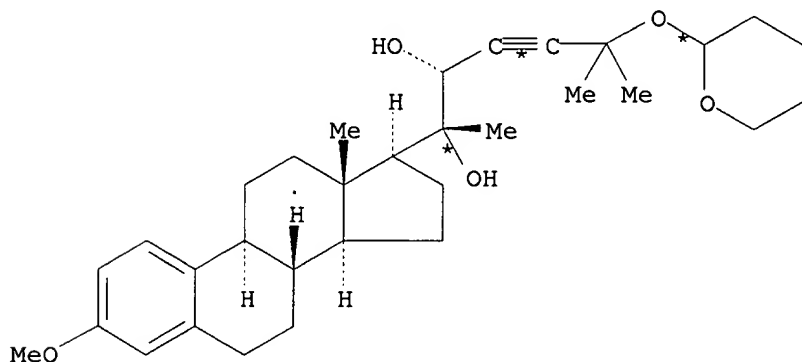
LANGUAGE: English

AB The addn. of LiC.tplbond.CCMe2O-THP (THP = tetrahydro-2H-pyran-2-yl) to
(20R)-20-hydroxypregnane-20-carboxaldehydes I and II in the absence and in
the presence of BF₃ afforded predominantly 20R,22R-diols III and IV or
20R,22S-diols V and VI, resp., characteristic of ecdysones.

RX(9) OF 53 ...R + Q ==> Z + AA



R



Q

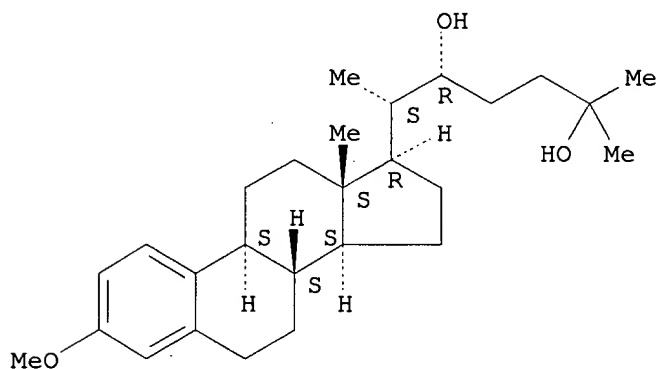
(9) →

=> s l1 and 19850804/ed
11811 19850804/ED
(850804/ED)
L11 1 L1 AND 19850804/ED

=> d

L11 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN 97452-85-2 REGISTRY
CN 19-Norcholesta-1,3,5(10)-triene-22,25-diol, 3-methoxy-, (22R)- (9CI) (CA
INDEX NAME)
FS STEREOSEARCH
MF C27 H42 O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

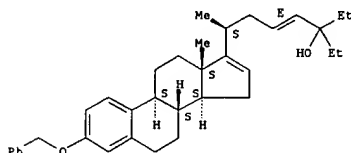
L6 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2003:263913 CAPLUS
 DOCUMENT NUMBER: 139:7056
 TITLE: Regio- and Stereoselective Ruthenium-Catalyzed Hydrovinylation of 1,3-Dienes: Application to the Generation of a 20(S) Steroidal Side Chain
 AUTHOR(S): He, Zhengjie; Yi, Chae S.; Donaldson, William A.
 CORPORATE SOURCE: Department of Chemistry, Marquette University, Milwaukee, WI, 53201-1881, USA
 SOURCE: Organic Letters (2003), 5(9), 1567-1569
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 139:7056

AB The addn. of ethylene to 1,3-dienes and 1-vinylcycloalkenes, catalyzed by two ruthenium complexes, proceeds in a regioselective fashion to afford 3-methyl-1,4-dienes as products. For example, cyclohexene 1 (R = H, CH=CH₂, R₁ = CH=CH₂) gives 1 (R₁ = CH=CH₂) in 57-62% yield. For a steroidal-based 1-vinylcycloalkene 11, the addn. is stereospecific, giving a product with a 20(S) configuration.

IT 533925-77-8P
 RI: SPN (Synthetic preparation); PREP (Preparation)
 (regio- and stereoselective ruthenium-catalyzed hydrovinylation of 1,3-dienes, vinylcycloalkenes, and steroidal diene)
 RN 533925-77-8 CAPLUS
 CN 4-Octen-3-ol, 3-ethyl-7-[3-(phenylmethoxy)estra-1,3,5(10),16-tetraen-17-yl]-, (4E,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
 Double bond geometry as shown.

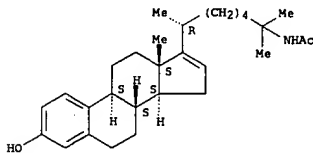


REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (synthesis of cholestane compds. with a c17-alkyl side chain and an arom. A-ring for use in cell modulating therapy)

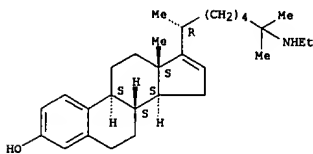
RN 305812-17-3 CAPLUS
 CN Acetamide, N-[(6R)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-18-4 CAPLUS
 CN 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-[5-(ethylamino)-5-methylhexyl]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-52-6 CAPLUS
 CN 19-Norcholesta-1,3,5(10)-trien-23-yne-3,25-diol (9CI) (CA INDEX NAME)

Absolute stereochemistry.

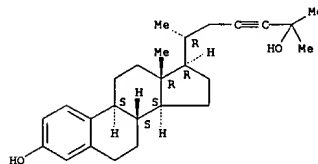
L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:814500 CAPLUS
 DOCUMENT NUMBER: 133:350395
 TITLE: Synthesis of cholestane compounds with a c17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy
 INVENTOR(S): Heese, Robert Henry; Setty, Sundara Katugam
 Srinivasasetty; Ramgopal, Malathi; Kugabaluooriar, Sanga
 PATENT ASSIGNEE(S): Marsden, John, Christopher, UK; Research Institute for Medicine and Chemistry Inc.
 SOURCE: ECT Int. Appl., 75 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000068246	A1	20001116	WO 2000-GB1813	20000511
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, FR, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1179005	A1	20020213	EP 2000-927569	20000511
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
ZA 2001009272	A	20021128	ZA 2001-9272	20011109
NO 2001005520	A	20020109	NO 2001-5520	20011112
PRIORITY APPLN. INFO.: GB 1999-10934 A 19990511				
WO 2000-GB1813 W 20000511				

OTHER SOURCE(S): MARPAT 133:350395
 AB Synthesis of cholestane compds. (I) [R1 and R2, which may be the same or different, = alkyl, alkenyl, alkynyl; R3 = Me having .alpha.- or .beta.-configuration; R4 = H or an etherifying or esterifying group; R5 = H, OH, alkoxy; X = OR4, wherein R4 is as defined above, or NR6R7 wherein R6 = H, aliph. or araliph. org. group, acyl group comprising aliph., araliph. or aryl org. group linked to the nitrogen atom by way of a carbonyl group; R7 = H, alkyl; Y = (un)substituted alkylene, alkenylene, alkynylene; dotted lines signify that double bonds may be present at the 16(17)-position and/or either at the 6(7)- and 8(9)-positions or at the 7(8)-position] is disclosed for modulation of cell growth and differentiation, while having low calcemic activity. Thus, I [R1, R2 = Me; R3 = .alpha.-Me; R4, R5 = H; X = NHAc; Y = (CH2)4; .DELTA.16 double bond] is prep. by reaction of 3-triisopropylsilyloxy-19-norchole-1,3,5(10),16-tetraene-24-bromide with acetonitrile followed by redn. of nitrile to amine, methylation of amine with Me lithium, acetylation of the amino with acetic anhydride and desilylation with TBAF.
 IT 305812-17-3P 305812-18-4P 305812-52-6P
 RI: BAC (Biological activity or effector, except adverse); BSU (Biological

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

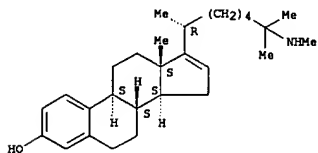


IT 305812-19-5P 305812-20-8P 305812-21-9P
 305812-22-0P 305812-23-1P 305812-24-2P
 305812-25-3P 305812-26-4P 305812-27-5P
 305812-28-6P 305812-29-7P 305812-30-0P
 305812-31-1P 305812-32-2P 305812-33-3P
 305812-34-4P 305812-35-5P 305812-36-6P
 305812-37-7P 305812-38-8P 305812-39-9P
 305812-40-2P 305812-41-3P 305812-42-4P
 305812-43-5P 305812-44-6P 305812-45-7P
 305812-46-8P 305812-47-9P 305812-48-0P
 305812-49-1P 305812-53-7P 305812-54-0P
 305812-55-9P 305812-56-0P 305812-57-1P
 305812-58-2P 305812-59-3P 305812-60-6P
 305812-61-7P 305812-62-8P 305812-63-9P
 305812-64-0P

RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (synthesis of cholestane compds. with a c17-alkyl side chain and an arom. A-ring for use in cell modulating therapy)

RN 305812-19-5 CAPLUS
 CN 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-[5-methyl-5-(methylamino)hexyl]-, (20R)- (9CI) (CA INDEX NAME)

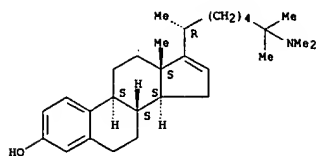
Absolute stereochemistry.



RN 305812-20-8 CAPLUS
 CN 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-[5-(dimethylamino)-5-methylhexyl]-, (20R)- (9CI) (CA INDEX NAME)

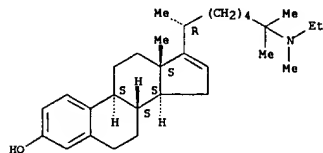
Absolute stereochemistry.

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



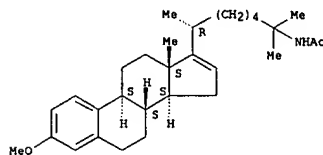
RN 305812-21-9 CAPLUS
CN 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-[(5-ethylmethylamino)-5-methylhexyl]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-22-0 CAPLUS
CN Acetamide, N-[(6R)-6-(3-methoxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

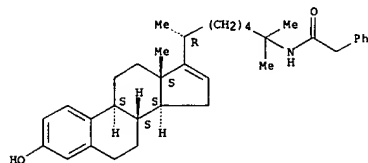


RN 305812-23-1 CAPLUS
CN Acetamide, N-[(6R)-6-(3-ethoxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

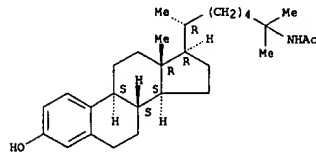
L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

Absolute stereochemistry.



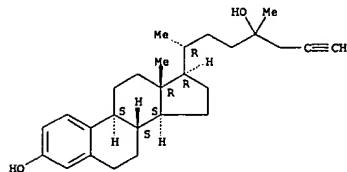
RN 305812-27-5 CAPLUS
CN Acetamide, N-[(6R)-6-(17.β)-3-hydroxyestra-1,3,5(10)-trien-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



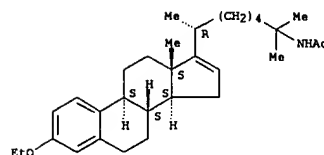
RN 305812-28-6 CAPLUS
CN 19,26,27-Trinorcholesta-1,3,5(10)-triene-3,24-diol, 24-(2-propynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



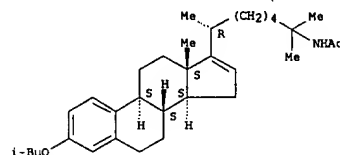
RN 305812-29-7 CAPLUS
CN 19,26,27-Trinorcholesta-1,3,5(10)-triene-3,24-diol, 2-methoxy-24-(2-propynyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



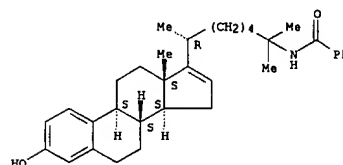
RN 305812-24-2 CAPLUS
CN Acetamide, N-[(6R)-1,1-dimethyl-6-[3-(2-methylpropoxy)estra-1,3,5(10),16-tetraen-17-yl]heptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-25-3 CAPLUS
CN Benzamide, N-[(6R)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

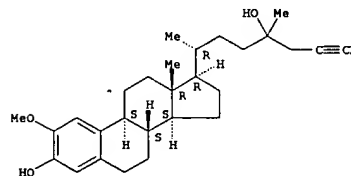
Absolute stereochemistry.



RN 305812-26-4 CAPLUS
CN Benzeneacetamide, N-[(6R)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

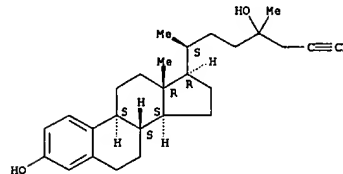
L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

Absolute stereochemistry.

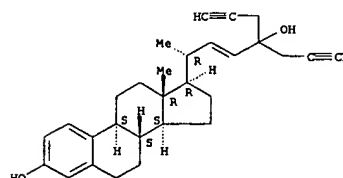


RN 305812-30-0 CAPLUS
CN 19,26,27-Trinorcholesta-1,3,5(10)-triene-3,24-diol, 24-(2-propynyl)-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



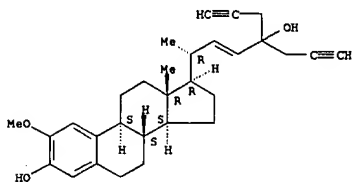
RN 305812-31-1 CAPLUS
CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-[3-hydroxy-3-(2-propynyl)-1-hexen-5-ynyl]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

RN 305812-32-2 CAPLUS
CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-[3-hydroxy-3-(2-propynyl)-1-hexen-5-

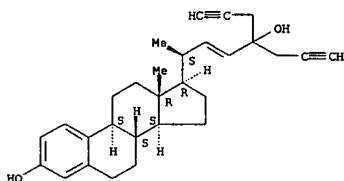
L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 ynyl]-2-methoxy-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.



RN 305812-33-3 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-[(3-hydroxy-3-(2-propynyl)-1-hexen-5-ynyl)-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.

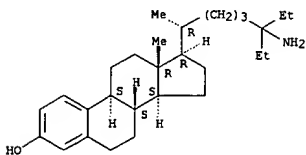


RN 305812-34-4 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-[(4-amino-4-ethyl-2-hexynyl)-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

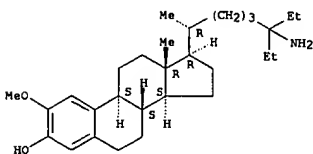
L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-[(4-amino-4-ethylhexyl)-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



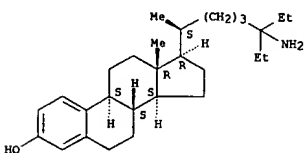
RN 305812-38-8 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-[(4-amino-4-ethylhexyl)-2-methoxy-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



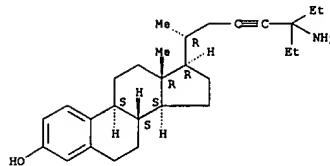
RN 305812-39-9 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-[(4-amino-4-ethylhexyl)-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



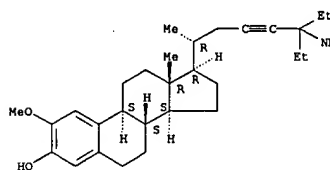
RN 305812-40-2 CAPLUS
 CN Acetamide, N-[(5R)-1,1-diethyl-5-[(17.beta.)-3-hydroxyestra-1,3,5(10)-trien-17-yl]-2-hexynyl]- (9CI) (CA INDEX NAME)

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



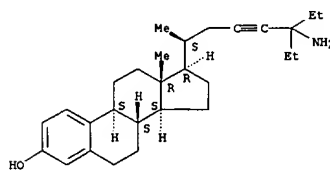
RN 305812-35-5 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-[(4-amino-4-ethyl-2-hexynyl)-2-methoxy-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



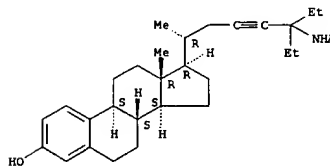
RN 305812-36-6 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-[(4-amino-4-ethyl-2-hexynyl)-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



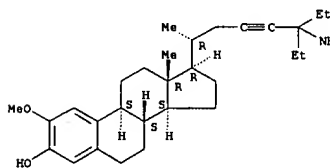
RN 305812-37-7 CAPLUS

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 Absolute stereochemistry.



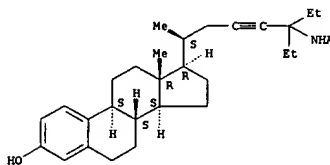
RN 305812-41-3 CAPLUS
 CN Acetamide, N-[(5R)-1,1-diethyl-5-[(17.beta.)-3-hydroxy-2-methoxyestra-1,3,5(10)-trien-17-yl]-2-hexynyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



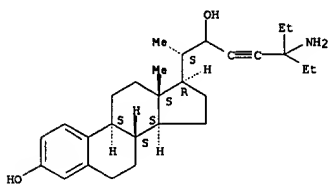
RN 305812-42-4 CAPLUS
 CN Acetamide, N-[(5S)-1,1-diethyl-5-[(17.beta.)-3-hydroxyestra-1,3,5(10)-trien-17-yl]-2-hexynyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



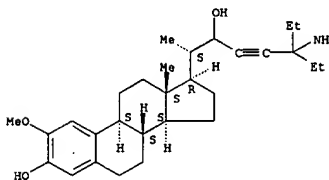
RN 305812-43-5 CAPLUS
 CN 19-Norpregna-1,3,5(10)-triene-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentynyl)-3-hydroxy-, (20S)- (9CI) (CA INDEX NAME)

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
Absolute stereochemistry.



RN 305812-44-6 CAPLUS
CN 19-Norpregna-1,3,5(10)-triene-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentynyl)-3-hydroxy-2-methoxy-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

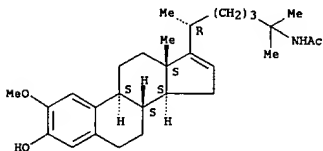


RN 305812-45-7 CAPLUS
CN 19-Norpregna-1,3,5(10)-triene-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentynyl)-3-hydroxy-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

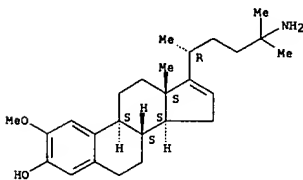
L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



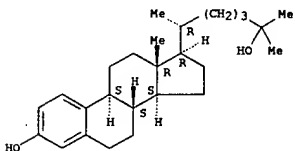
RN 305812-49-1 CAPLUS
CN 19,26,27-Trinorergosta-1,3,5(10),16-tetraen-3-ol, 24-amino-2-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



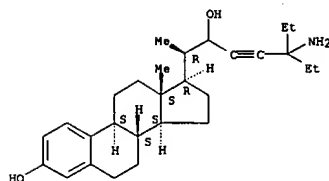
RN 305812-53-7 CAPLUS
CN 19-Norcholesta-1,3,5(10)-triene-3,25-diol (9CI) (CA INDEX NAME)

Absolute stereochemistry.



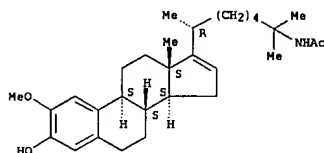
RN 305812-54-8 CAPLUS
CN 19-Norcholesta-1,3,5(10)-triene-3,25-diol, 2-methoxy- (9CI) (CA INDEX NAME)

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



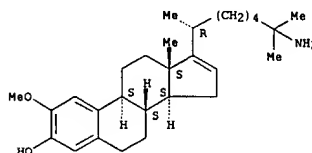
RN 305812-46-8 CAPLUS
CN Acetamide, N-[(6R)-6-(3-hydroxy-2-methoxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



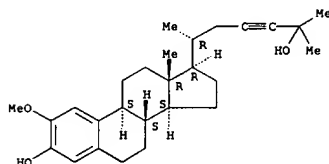
RN 305812-47-9 CAPLUS
CN 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-(5-amino-5-methylhexyl)-2-methoxy-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



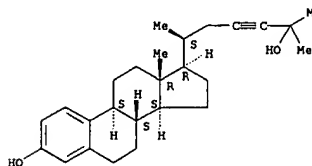
RN 305812-48-0 CAPLUS
CN Acetamide, N-(3-hydroxy-2-methoxy-19-norcholesta-1,3,5(10),16-tetraen-25-

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
Absolute stereochemistry.



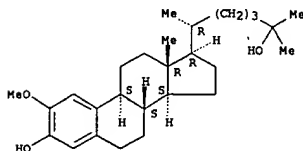
RN 305812-55-9 CAPLUS
CN 19-Norcholesta-1,3,5(10)-triene-3,25-diol, 2-methoxy-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-56-0 CAPLUS
CN 19-Norcholesta-1,3,5(10)-triene-3,25-diol, 2-methoxy-, (9CI) (CA INDEX NAME)

Absolute stereochemistry.

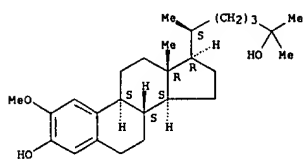


RN 305812-57-1 CAPLUS
CN 19-Norcholesta-1,3,5(10)-triene-3,25-diol, 2-methoxy-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

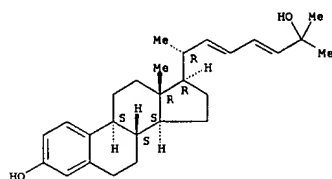
L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

(Continued)



RN 305812-58-2 CAPLUS

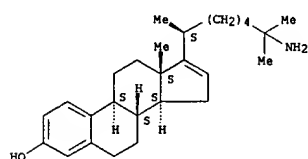
CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(5-hydroxy-5-methyl-1,3-hexadienyl)-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

RN 305812-59-3 CAPLUS

CN 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-(5-amino-5-methylhexyl)-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-60-6 CAPLUS

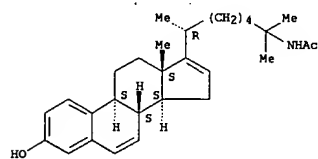
CN Acetamide, N-[(6S)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

(Continued)

CN Acetamide, N-[(6R)-6-(3-hydroxyestra-1,3,5(10),6,16-pentaen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

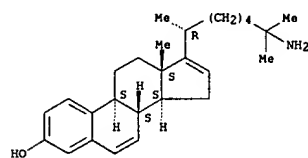
Absolute stereochemistry.



RN 305812-64-0 CAPLUS

CN 19-Norpregna-1,3,5(10),6,16-pentaen-3-ol, 20-(5-amino-5-methylhexyl)-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 305813-30-3P 305813-32-5P 305813-36-9P

305813-38-1P 305813-41-6P 305813-43-8P

305813-44-9P 305813-46-1P 305813-47-2P

305813-51-8P 305813-53-0P 305813-55-2P

305813-56-3P 305813-58-5P 305813-59-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of cholestane compds. with a c17-alkyl side chain and an arom. A-ring for use in cell modulating therapy)

RN 305813-30-3 CAPLUS

CN 19-Norpregna-1,3,5(10),16-tetraene-20-pentanamine, .alpha.,.alpha.-dimethyl-3-[[tris(1-methylethyl)silyl]oxy]-, (20R)- (9CI) (CA INDEX NAME)

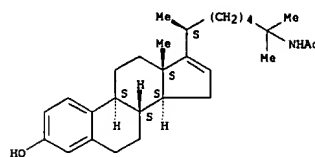
Absolute stereochemistry.

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

(Continued)

dimethylheptyl]- (9CI) (CA INDEX NAME)

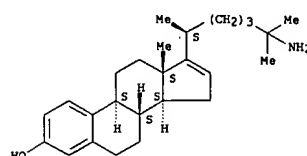
Absolute stereochemistry.



RN 305812-61-7 CAPLUS

CN 19-Norcholesta-1,3,5(10),16-tetraen-3-ol, 25-amino-, (20S)- (9CI) (CA INDEX NAME)

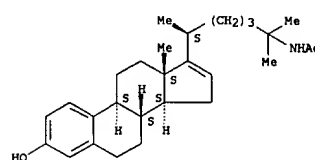
Absolute stereochemistry.



RN 305812-62-8 CAPLUS

CN Acetamide, N-[(20S)-3-hydroxy-19-norcholesta-1,3,5(10),16-tetraen-25-yl]- (9CI) (CA INDEX NAME)

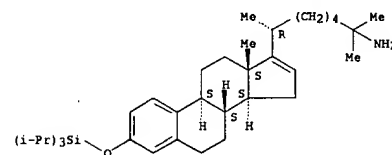
Absolute stereochemistry.



RN 305812-63-9 CAPLUS

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

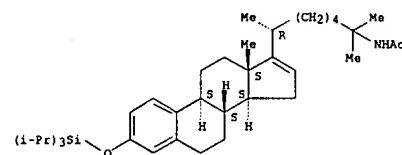
(Continued)



RN 305813-32-5 CAPLUS

CN Acetamide, N-[(6R)-1,1-dimethyl-6-[3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10),16-tetraen-17-yl]heptyl]- (9CI) (CA INDEX NAME)

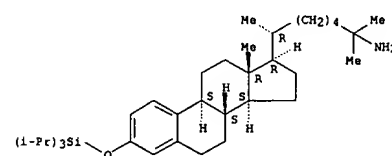
Absolute stereochemistry.



RN 305813-36-9 CAPLUS

CN 19-Norpregna-1,3,5(10)-triene-20-pentanamine, .alpha.,.alpha.-dimethyl-3-[[tris(1-methylethyl)silyl]oxy]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

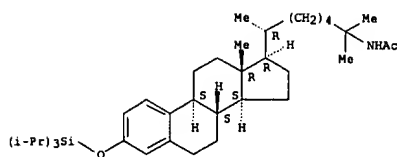


RN 305813-38-1 CAPLUS

CN Acetamide, N-[(6R)-1,1-dimethyl-6-[(17.beta.)-3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10)-trien-17-yl]heptyl]- (9CI) (CA INDEX NAME)

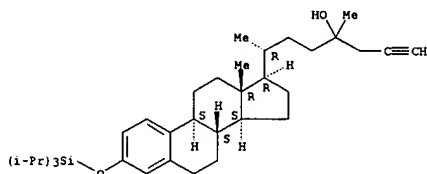
Absolute stereochemistry.

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



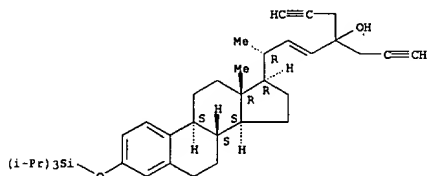
RN 305813-41-6 CAPLUS
CN 19,26,27-Trinorcholesta-1,3,5(10)-trien-24-ol, 24-(2-propynyl)-3-[[tris(1-methylethyl)silyl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

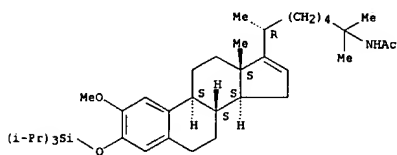


RN 305813-43-8 CAPLUS
CN 5-Octen-1-yn-4-ol, 4-(2-propynyl)-7-[(17.beta.)-3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10)-trien-17-yl]-, (7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

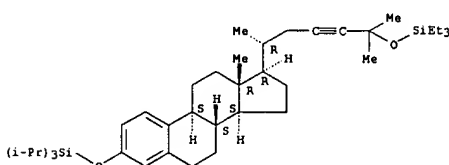


L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



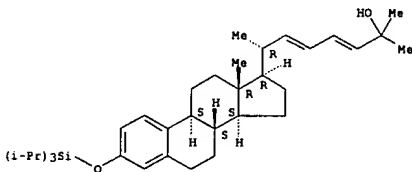
RN 305813-51-8 CAPLUS
CN Silane, [[25-[[triethylsilyl]oxy]-19-norcholesta-1,3,5(10)-trien-23-yn-3-yl]oxy]tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305813-53-0 CAPLUS
CN 3,5-Octadien-2-ol, 2-methyl-7-[(17.beta.)-3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10)-trien-17-yl]-, (7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

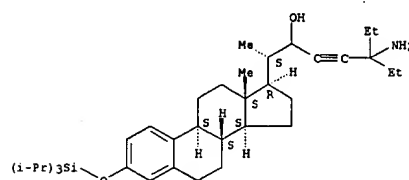


RN 305813-55-2 CAPLUS
CN 19-Norpregna-1,3,5(10),16-tetraene-20-pentanamine, .alpha.,.alpha.-dimethyl-3-[[tris(1-methylethyl)silyl]oxy]-, (20S)- (9CI) (CA INDEX NAME)

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

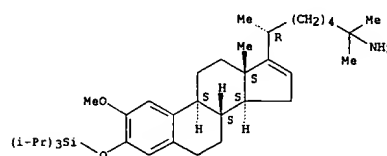
RN 305813-44-9 CAPLUS
CN 19-Norpregna-1,3,5(10)-trien-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentynyl)-3-[[tris(1-methylethyl)silyl]oxy]-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305813-46-1 CAPLUS
CN 19-Norpregna-1,3,5(10),16-tetraene-20-pentanamine, 2-methoxy-.alpha.,.alpha.-dimethyl-3-[[tris(1-methylethyl)silyl]oxy]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



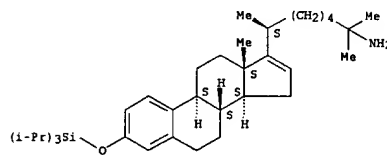
RN 305813-47-2 CAPLUS
CN Acetamide, N-[(6R)-6-[2-methoxy-3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10),16-tetraen-17-yl]-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



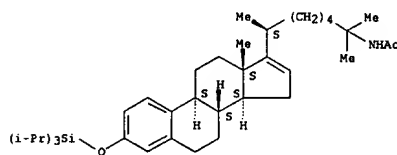
L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

Absolute stereochemistry.



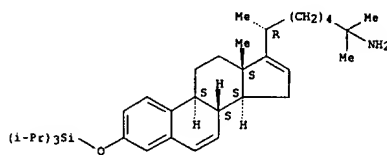
RN 305813-56-3 CAPLUS
CN Acetamide, N-[(6S)-1,1-dimethyl-6-[3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10),16-tetraen-17-yl]heptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305813-58-5 CAPLUS
CN 19-Norpregna-1,3,5(10),6,16-pentaene-20-pentanamine, .alpha.,.alpha.-dimethyl-3-[[tris(1-methylethyl)silyl]oxy]-, (20R)- (9CI) (CA INDEX NAME)

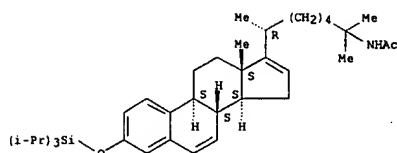
Absolute stereochemistry.



RN 305813-59-6 CAPLUS
CN Acetamide, N-[(6R)-1,1-dimethyl-6-[3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10),6,16-pentaen-17-yl]heptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



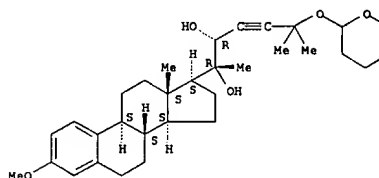
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1985:471583 CAPLUS
 DOCUMENT NUMBER: 103:71583
 TITLE: A stereoselective synthesis of 1,2-diols from
 .alpha.-hydroxyaldehydes
 AUTHOR(S): Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.;
 Russell, Graeme B.; Horn, Dennis H. S.
 CORPORATE SOURCE: Dep. Chem., Univ. Wyoming, Laramie, WY, 82071, USA
 SOURCE: Tetrahedron Letters (1985), 26(9), 1189-92
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English

OTHER SOURCE(S): CASREACT 103:71583
 AB The addn. of LiC.tpbond.CMe2O-THP (THP = tetrahydro-2H-pyran-2-yl) to
 (20R)-20-hydroxypregnane-20-carboxaldehydes I and II in the absence and in
 the presence of BF3 afforded predominantly 20R,22R-diols III and IV or
 20R,22S-diols V and VI, resp., characteristic of ecdysones.
 IT 97452-83-OP 97452-84-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and hydrolysis-hydrogenation of)
 RN 97452-83-D CAPLUS
 CN 19-Norcholesta-1,3,5(10)-trien-23-yne-20,22-diol, 3-methoxy-25-
 [(tetrahydro-2H-pyran-2-yl)oxy]-, (22R)- (9CI) (CA INDEX NAME)

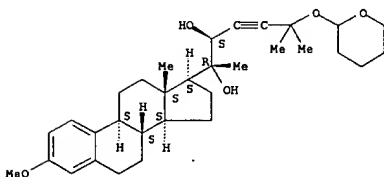
Absolute stereochemistry.



RN 97452-84-1 CAPLUS
 CN 19-Norcholesta-1,3,5(10)-trien-23-yne-20,22-diol, 3-methoxy-25-
 [(tetrahydro-2H-pyran-2-yl)oxy]-, (22S)- (9CI) (CA INDEX NAME)

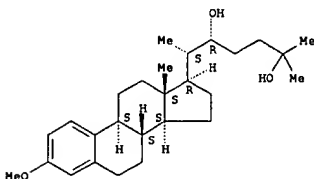
Absolute stereochemistry.

L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



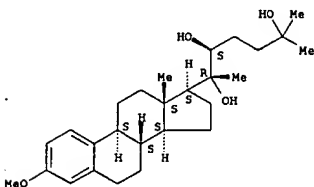
IT 97452-85-2P 97452-86-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 97452-85-2 CAPLUS
 CN 19-Norcholesta-1,3,5(10)-triene-22,25-diol, 3-methoxy-, (22R)- (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.



RN 97452-86-3 CAPLUS
 CN 19-Norcholesta-1,3,5(10)-triene-20,22,25-triol, 3-methoxy-, (22S)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

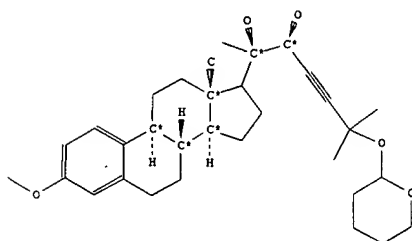
09/926,491

Page 9

=> d all 1-4

L7 ANSWER 1 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 4728055
CAS Reg. No. (RN): 97452-83-0, 97452-84-1
Chemical Name (CN): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol
Autonom Name (AUN): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol
Molec. Formula (MF): C32 H46 O5
Molecular Weight (MW): 510.71
Lawson Number (LN): 17122, 6760, 289
File Segment (FS): Stereo compound
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 4263612
Tautomer ID (TAUTID): 4567456
Beilstein Citation (BSO): 6-17
Entry Date (DED): 1991/12/02
Update Date (DUPD): 1991/12/02



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
RN	CAS Registry Number	2
CN	Chemical Name	1
AUN	Autonomname	1

L7 ANSWER 1 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

(Continued)

Reactant (.RCT): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol
Product BRN (.PBRN): 4722039
Product (.PRO): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3,6-triol
No. of React. Details (.NVAR): 1

Reaction Details:

RX
Reaction RID (.RID): 2742338.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 90 percent (BRN=4722039)
Reagent (.RGT): 70 percent HClO4
Solvent (.SOL): H2O, methanol
Reference(s):
1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.; Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

Reaction:

RX
Reaction ID (.ID): 2742337
Reactant BRN (.RBRN): 4728055
Reactant (.RCT): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol
Product BRN (.PBRN): 4722039
Product (.PRO): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3,6-triol
No. of React. Details (.NVAR): 1

Reaction Details:

RX
Reaction RID (.RID): 2742337.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 90 percent (BRN=4722038)
Reagent (.RGT): 70 percent HClO4
Solvent (.SOL): H2O, methanol
Reference(s):
1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.; Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

L7 ANSWER 1 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

(Continued)

Code	Name	Occurrence
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	3
RXREA	Substance is Reaction Reactant	2
RXPRO	Substance is Reaction Product	1

Reaction:

RX
Reaction ID (.ID): 2442472
Reactant BRN (.RBRN): 4525023, 4133964
Reactant (.RCT): 2-hydroxy-2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-propionaldehyde, C10H15BrMgO2
Product BRN (.PBRN): 4728055, 4728054
Product (.PRO): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol, 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol
No. of React. Details (.NVAR): 1

Reaction Details:

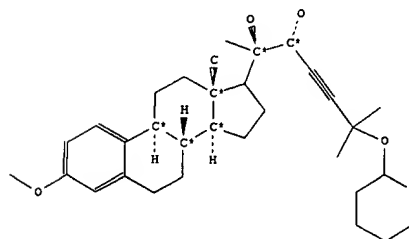
RX
Reaction RID (.RID): 2442472.1
Reaction Classification (.CL): Preparation
Solvent (.SOL): tetrahydrofuran
Temperature (.T): -26 Cel
Note(s) (.COM): Yield given. Yields of byproduct given
Reference(s):
1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.; Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

Reaction:

RX
Reaction ID (.ID): 2742338
Reactant BRN (.RBRN): 4728055

L7 ANSWER 2 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 4728054
CAS Reg. No. (RN): 97452-83-0, 97452-84-1
Chemical Name (CN): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol
Autonom Name (AUN): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol
Molec. Formula (MF): C32 H46 O5
Molecular Weight (MW): 510.71
Lawson Number (LN): 17122, 6760, 289
File Segment (FS): Stereo compound
Compound Type (CTYPE): heterocyclic
Constitution ID (CONSID): 4263612
Tautomer ID (TAUTID): 4567455
Beilstein Citation (BSO): 6-17
Entry Date (DED): 1991/12/02
Update Date (DUPD): 1991/12/02



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
RN	CAS Registry Number	2
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	1

L7 ANSWER 2 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

(Continued)

CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Reaction:

RX

Reaction ID (.ID):	2442472
Reactant BRN (.RBRN):	4525023, 4133964
Reactant (.RCT):	2-hydroxy-2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-propionaldehyde, C10H15BrMgO2
Product BRN (.PBRN):	4728055, 4728054
Product (.PRO):	2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol, 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol

No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID):	2442472.1
Reaction Classification (.CL):	Preparation
Solvent (.SOL):	tetrahydrofuran
Temperature (.T):	-26 Cel
Note(s) (.COM):	Yield given. Yields of byproduct given
Reference(s):	1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.; Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

L7 ANSWER 3 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

(Continued)

CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
NMR	Nuclear Magnetic Resonance	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Nuclear Magnetic Resonance:

NMR

Description (.KW):	Chemical shifts
Nucleus (.NUC):	13C
Solvents (.SOL):	pyridine-d5
Reference(s):	1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.; Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

Reaction:

RX

Reaction ID (.ID):	2737115
Reactant BRN (.RBRN):	4722039
Reactant (.RCT):	2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-hept-4-yne-2,3,6-triol
Product BRN (.PBRN):	4719751
Product (.PRO):	2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-heptane-2,3,6-triol

No. of React. Details (.NVAR): 1

Reaction Details:

RX

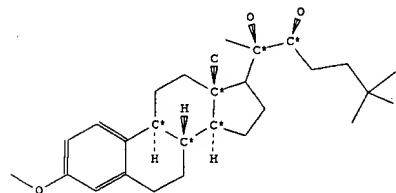
Reaction RID (.RID):	2737115.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	H2
Catalyst (.CAT):	PtO2
Reference(s):	1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.; Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

L7 ANSWER 3 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN):	4719751
Beilstein Pref. RN (BPR):	97452-86-3
CAS Reg. No. (RN):	97452-86-3
Chemical Name (CN):	2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-heptane-2,3,6-triol

Autonom Name (AUN):

Molec. Formula (MF):	C27 H42 O4
Molecular Weight (MW):	430.63
Lawson Number (LN):	6704, 289
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	4257631
Tautomer ID (TAUTID):	4555354
Beilstein Citation (BSO):	6-06
Entry Date (DED):	1991/12/02
Update Date (DUPD):	1993/03/20



Field Availability:

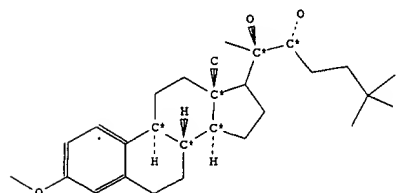
Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1

L7 ANSWER 4 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN):	4719750
Beilstein Pref. RN (BPR):	97452-86-3
CAS Reg. No. (RN):	97452-86-3
Chemical Name (CN):	2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-heptane-2,3,6-triol

Autonom Name (AUN):

Molec. Formula (MF):	C27 H42 O4
Molecular Weight (MW):	430.63
Lawson Number (LN):	6704, 289
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	4257631
Tautomer ID (TAUTID):	4555353
Beilstein Citation (BSO):	6-06
Entry Date (DED):	1991/12/02
Update Date (DUPD):	1993/03/20



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1

L7 ANSWER 4 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

UPD	Update Date	1
NMR	Nuclear Magnetic Resonance	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Nuclear Magnetic Resonance:

NMR

Description (.KW):	Chemical shifts
Nucleus (.NUC):	¹³ C
Solvents (.SOL):	pyridine-d5

Reference(s):

1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.; Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

Reaction:

RX

Reaction ID (.ID):	2737114
Reactant BRN (.RBRN):	4722038
Reactant (.RCT):	2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-17-yl)-6-methylhept-4-yne-2,3,6-triol
Product BRN (.PBRN):	4719750
Product (.PRO):	2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-17-yl)-6-methylheptane-2,3,6-triol

No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID):	2737114.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	H2
Catalyst (.CAT):	PtO2

Reference(s):

1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.; Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

=> d ibib ab fqhit 1-14

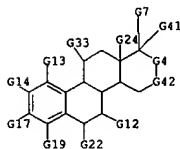
L9 ANSWER 1 OF 14 MARPAT COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 138:73420 MARPAT
 TITLE: Preparation of anti-estrogenic steroids, and associated pharmaceutical compositions and methods of use
 INVENTOR(S): Tanabe, Masato; Peters, Richard H.; Chao, Wan-Ru; Jong, Ling
 PATENT ASSIGNEE(S): SRI International, USA
 SOURCE: U.S., 50 pp., Cont. of U.S. Ser. No. 220,408.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 4
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6503896	B1	20030107	US 2001-872826	20010531
US 6054446	A	20000425	US 1997-998877	19971224
EP 1310509	A2	20030514	EP 2003-183	19981223

R: DE, FR, GB, IT, NL
 US 6281205 B1 20010828
 US 1998-220408 19981224
 US 1997-998877 19971224
 US 1998-220408 19981224
 EP 1998-964882 19981223

AB Steroid derivs., such as I and II [R = C, N; dashed lines = optional double bonds; X, X1 = hydrocarbonyl, generally including at least one O, S, N atom in the form of -O-, -S-, -NH- or, -N(alkyl)-linkage; XX1 = heterocyclic ring; R1 = H, alkyl; R2 = H, OH, alkyl, alkoxy, thioalkyl; R3-R5, R7, R9 = H, alkyl; R6 = H, alkyl, acyl; R8 = H, OH, alkoxy; R10 = Me, Et; R20 = -CH(CH2)m-O-L-(CH2)p-NR21R22, -CH(CH2)m-O-p-(sub)C6H4-(CH2)p-NR21R22; m = 0-5; p = 0-6; L = cyclic or heterocyclic ring; R21, R22 = alkyl; R21R22 = cycloalkyl, heterocycloalkyl, or a pharmaceutically acceptable salt thereof, were prepd to treat a variety of disorders, particularly estrogen-dependent disorders including prostatic cancer. Thus, (E)-3-hydroxy-21-(2'-(piperazinyl)ethoxy)-19-norpregna-1,3,5(10),17(20)-tetraene (III) was prepd. via a multistep synthetic sequence starting from estrone, vinylmagnesium bromide, and 1-(2-hydroxyethyl)piperazine. III exhibited 100% antiestrogenic activity against Human Ishikawa cells at 10 μ M concn. Therapeutic methods and pharmaceutical compns. were also provided.

FIGURE 3



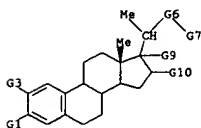
L9 ANSWER 2 OF 14 MARPAT COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 137:370278 MARPAT
 TITLE: Preparation of substituted pregna-1,3,5(10)-triene derivatives for pharmaceutical use
 INVENTOR(S): Hesse, Robert Henry; Setty, Sundara Katugam
 Sriniwasasetty; Pechet, Maurice Murdoch; Gile, Michael
 PATENT ASSIGNEE(S): Marsden, John Christopher, UK; Research Institute for Medicine and Chemistry Inc.
 SOURCE: PCT Int. Appl., 28 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002092100	A1	20021121	WO 2002-GB2210	20020513

V: AE, AG, AL, AM, AT, AU, AZ, BA, BE, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, C2, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

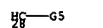
PRIORITY APPLN. INFO.: US 2001-290013P 20010511
 AB Pregna-1,3,5(10)-triene derivs., such as I [R1 = H, hydroxy protecting group; R2 = OH, CHO, alkoxy, alkenyl, alkyl, etc.; R3 = α -, β -, γ -Me; X = C1-3 alkylene group, bond; Y = C(R4)(R5)NR6R7; R4, R5 = H, alkyl, alkenyl and alkynyl groups, such that the total carbon content of R4 and R5 does not exceed three atoms; R6 = H, aliph. or araliph. org. group, acyl, etc.; C16-C17 = satd., unsatd.], were prepd. for a variety of therapeutic uses, such as modulating cell activity, including antiproliferative and antiangiogenic effects. Thus, pregna-1,3,5(10)-triene derivs. II (Y = NH2, NHCOMe) were prepd. via a multistep synthetic series starting from 2-methoxy-3-[[tris(1-methylethyl)silyl]oxy]-estra-1,3,5(10)-trien-17-one and ethyltriphenylphosphonium bromide. Pharmaceutical compns. of the prepd. compds. were discussed, but specific pharmaceutical activity testing data was not presented.

FIGURE 1

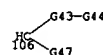


G1 = OH
 G3 = OH
 G6 = alkylene<(1-3)>
 G7 = 30

L9 ANSWER 1 OF 14 MARPAT COPYRIGHT 2003 ACS on STN (Continued)
 G4 = 28



G17 = OH
 G24 = Me
 G41 = 106



G43 = Ak (50)
 G45 = O
 G47 = alkyl<(1-24)> (50)
 DER: or pharmaceutically acceptable salts or esters
 MPL: disclosure
 NTE: oxo substitution also disclosed

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 14 MARPAT COPYRIGHT 2003 ACS on STN (Continued)



G8 = alkyl<(1-3)>
 G13 = NH2
 MPL: claim 1
 NTE: total carbon carbon content of G8 does not exceed three atoms
 NTE: substitution is restricted

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

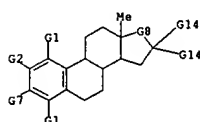
L9 ANSWER 3 OF 14 MARPAT COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 137:47357 MARPAT
 TITLE: Preparation of 2-methoxyestradiol derivatives as antiangiogenic agents
 INVENTOR(S): Agoston, Gregory E.; Shah, Jamshed H.; Hunsucker, Kimberly A.; Pribluda, Victor S.; Lavallee, Theresa M.; Green, Shawn J.; Herbstritt, Christopher J.; Zhan, Xiaoguo H.; Treston, Anthony M.
 PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 37 pp., Cont.-in-part of U. S. Ser. No. 933,894.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002082433	A1	20020627	US 2001-939208	20010824
PRIORITY APPLN. INFO.:			US 2000-641327	20000818
			US 2000-253385P	20001127
			US 2000-255302P	20001213
			US 2001-278250P	20010323
			US 2001-933894	20010821

AB 2-Methoxyestradiol derivs. of formula I [R1, R4 = H, halo, CN, alkyl, OH, NH2, etc.; R2 = N3, CN, OMe, alkenyl, alkynyl, alkoxy, NH2, etc.; R3 = OH, OR; R5 = alkyl, alkenyl, (di)alkylamino, OH, alkylene, etc.; R6, R7 = H, alkyl, alkenyl, alkynyl, halo, etc.] are prepd. for treating mammalian disease characterized by undesirable angiogenesis. Thus, II was prepd. from 2-methoxyestradiol and propyltriphenylphosphonium bromide. The IC50 of II against MDA-MB-231 breast tumor cells was 51.31 .mu.M.

MSTR 1



G2 = alkoxy<(-10)> (SO (1-) F)
 G7 = OH
 G8 = 53

HC—G13

G13 = alkyl<(1-10)> (SO (1-) G21)
 G21 = CF3 / OH
 MPL: claim 1

L9 ANSWER 3 OF 14 MARPAT COPYRIGHT 2003 ACS on STN (Continued)

NTE: additional double bond formation also claimed

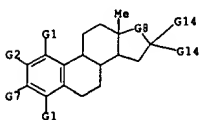
L9 ANSWER 4 OF 14 MARPAT COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 137:6309 MARPAT
 TITLE: Preparation of 2-methoxyestradiol analogs as antiangiogenic agents
 INVENTOR(S): Agoston, Gregory; Shah, Jamshed H.; Hunsucker, Kimberly A.; Pribluda, Victor; Lavallee, Theresa M.; Green, Shawn J.; Herbstritt, Christopher J.; Zhan, Xiaoguo H.; Treston, Anthony
 PATENT ASSIGNEE(S): Extramed, Inc., USA
 SOURCE: PCT Int. Appl., 86 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002042319	A2	20020530	WO 2001-US26490	20010824
WO 2002042319	A3	20030313		
V: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2001088386	A5	20020603	AU 2001-88386	20010824
EP 1343803	A2	20030917	EP 2001-968112	20010824
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
PRIORITY APPLN. INFO.:			US 2000-253385P	20001127
			US 2000-255302P	20001213
			US 2001-278250P	20010323
			US 2001-933894	20010821
			WO 2001-US26490	20010824

AB 2-Methoxyestradiol analogs, such as I [R1, R3 = H, halo, CN, alkyl, OH, CH2OH, NH2, alkylamino; R2 = N3, CN, C.tpbond.CR, C=CHR, C.tpbond.CH, OR, amino; R = H, alkyl; Z = COH, COAc; dashed bond = single bond or double bond; R6 = H, OH, O, oxime, amino, alkyl, alkenyl; R4, R5 = H, alkyl, alkenyl, alkynyl], were prepd. for treating mammalian disease characterized by undesirable angiogenesis. Thus, 2-methoxyestradiol analog II was prepd. by the reaction of methyltriphenylphosphonium bromide and 2-methoxyestrone. In vitro evaluation against MDA-MB-231 breast tumor cells and HUVEC endothelial cells, II showed IC50 0.24+-0 and 0.19+-0.19 resp.

MSTR 1



L9 ANSWER 4 OF 14 MARPAT COPYRIGHT 2003 ACS on STN (Continued)

G2 = alkoxy<(-10)> (SO (1-) F)
 G7 = OH
 G8 = 53

HC—G13

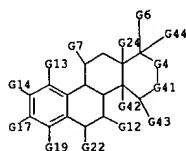
G13 = alkyl<(1-10)> (SO (1-) G21)
 G21 = CF3 / OH
 MPL: claim 1
 NTE: additional double bond formation also claimed

L9 ANSWER 5 OF 14 MARPAT COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 136:232440 MARPAT
 TITLE: Preparation of novel anti-estrogenic steroids
 INVENTOR(S): Tanabe, Masatos; Peters, Richard H.; Chao, Wan-cu;
 Jong, Ling
 PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 56 pp., Cont.-in-part of U.S.
 6,281,205.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 4
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002032180	A1	20020314	US 2001-872825	20010531
US 6548491	B2	20030415		
US 6054446	A	20000425	US 1997-998877	19971224
EP 1310509	A2	20030514	EP 2003-183	19981223
R: DE, FR, GB, IT, NL				
US 6281205	B1	20010828	US 1998-220408	19981224
US 2003153543	A1	20030814	US 2002-327401	20021219
PRIORITY APPLN. INFO.:			US 1997-998877	19971224
			US 1998-220408	19981224
			EP 1998-964882	19981223
			US 2001-872825	20010531

AB Novel antiestrogenic compds., e.g. of formula I [X = hydrocarbon contg. O, S or N, etc.; X1 = H, hydrocarbon contg. O, S or N, etc.; X11 = heterocycle; Y = C, H, RI = H, alkyl, halo, etc.; R2 = H, OH, alkyl, alkenyl, aryl, etc.; R3 = H, OH, CN, alkyl, etc.; R4 = H, alkyl; R5 = H, alkoxy, halo, CN, etc.; R6 = H, alkyl, acyl, SO2NH2; R7 = H, halo, nitro, CHO, allyl, etc.; R8 = H, OH, etc.; R9 = H, alkyl; R10 = Me, Et], are prepd. which are useful to treat a variety of disorders, particularly estrogen-dependent disorders. Preferred compds. have a 1,3,5-estratriene nucleus, and are substituted at the C-17 or C-11 position with a mol. moiety which renders the compds. effective to competitively block the binding of estrogen to its receptor. Therapeutic methods and pharmaceutical compds. are provided as well. Thus, II citrate salt was prepd. from 7.alpha.-methyl-17.beta.-hydroxyethyl-1,3,5-estratrien-3-ol, vanillin and diethylamine. II citrate salt showed significant growth suppressive activity against MCF-7 tumor in mice at 10 mg/kg/day.

MSTR 3

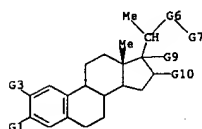


L9 ANSWER 6 OF 14 MARPAT COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 135:358085 MARPAT
 TITLE: Preparation of 2-substituted pregna-1,3,5(10)-triene and chola-1,3,5(10)-triene derivatives with antiproliferative and antiangiogenic activity
 INVENTOR(S): Hesse, Robert Henry; Setty, Sundara Katugam
 Srinivasasetty; Pechet, Maurice Murdoch; Gile, Michael
 PATENT ASSIGNEE(S): Marsden, John Christopher, UK; Research Institute for
 Medicine and Chemistry Inc.
 SOURCE: PCT Int. Appl., 40 pp.
 CODEN: PXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001085755	A1	20011115	WO 2001-GB2103	20010511
R: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, EG, ES, FI, FR, GB, GD, GE, GH, GM, GR, GU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, NZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BG, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1287017	A1	20030305	EP 2001-928120	20010511
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
NO 2002005392	A	20030109	NO 2002-5392	20021111
US 2003158167	A1	20030821	US 2003-275257	20030313
PRIORITY APPLN. INFO.:			US 2000-203462P	20000511
			WO 2001-GB2103	20010511

AB Compds. of formula I [R1 = H, protecting group; R2 = OH, alkoxy, CHO, alkenyl, etc.; X = alkylene, bond; Y = CHO, (substituted) CH2OH, etc.] are prepd. which exhibit potent cell modulating activity, including antiproliferative and antiangiogenic effects. Thus, 2-methoxy-3-triisopropylsilyloxy-19-norpregn-1,3,5(10),17(20)2-tetraene (prepn. given) is reacted with Me acrylate, reduced with LiAlH4, and desilylated with TBAF to give II.

MSTR 1



G1 = OH
 G3 = OH
 G6 = alkylene<(1-3)>

L9 ANSWER 5 OF 14 MARPAT COPYRIGHT 2003 ACS on STN (Continued)

G3 = 23



G4 = 28



G17 = OH
 G24 = Me
 G25 = Ak (SR (1-) G26)
 G27 = O
 G31 = alkyl<(1-24)>
 MPL: claim 20
 NTE: , or pharmaceutically acceptable salts or esters

L9 ANSWER 6 OF 14 MARPAT COPYRIGHT 2003 ACS on STN (Continued)

G7 = 30



G8 = alkyl<(1-3)>
 MPL: claim 1
 NTE: total carbon carbon content of G8 does not exceed three atoms
 NTE: substitution is restricted

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 7 OF 14 MARPAT COPYRIGHT 2003 ACS ON STN
 ACCESSION NUMBER: 135:195698 MARPAT
 TITLE: Preparation of anti-estrogenic steroids, and associated pharmaceutical compositions and methods of use
 INVENTOR(S): Tanabe, Masato; Peters, Richard H.; Chao, Wan-rui; Jong, Ling
 PATENT ASSIGNEE(S): Sri International, USA
 SOURCE: U.S., 50 pp., Cont.-in-part of U.S. 6,054,446.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 4
 PATENT INFORMATION:

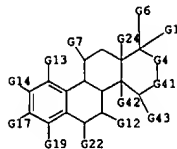
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6281205	B1	20010828	US 1998-220408	19981224
US 6054446	A	20000425	US 1997-998877	19971224
EP 1310509	A2	20030514	EP 2003-183	19981223
R: DE, FR, GB, IT, NL				
US 2002032180	A1	20020314	US 2001-872825	20010531
US 6548491	B2	20030415		
US 6503896	B1	20030107	US 2001-872826	20010531
US 2002032181	A1	20020314	US 2001-918890	20010730
US 6455517	B2	20020924		
US 2003153543	A1	20030814	US 2002-327401	20021219

PRIORITY APPLN. INFO.:

AB Novel antiestrogenic compds. are prepd. which are useful to treat a variety of disorders, particularly estrogen-dependent disorders. Preferred compds. have a 1,3,5(10)-estratriene nucleus, and are substituted at the C-17 or C-11 position with a mol. moiety which renders the compds. effective to competitively block the binding of estrogen to its receptor. Particularly preferred compds. are 17-desoxy-1,3,5(10)-estratrienes, e.g. of formula I [R1 = H, alkoxy, halo, CN, etc.; R2 = H, OH, alkyl, etc.; R3 = H, alkyl, acyl, SO2NH2, etc.; R4, R5 = H, alkyl, heterocyclyl, etc.; L = (substituted) five- or six-membered cyclic moiety; m = 1-6; p = 0-6]. Thus, II citrate salt was prepd. and showed strong growth inhibitory activity against MCF-7 human mammary tumor at 10 mg/kg/day. Therapeutic methods and pharmaceutical compns. are provided as well.

MYST 1

L9 ANSWER 7 OF 14 MARPAT COPYRIGHT 2003 ACS ON STN (Continued)



G3 = 23



G4 = 28



G17 = OH
 G24 = Me
 G25 = Ak (SR (1-24))
 G27 = O
 G31 = alkyl<(1-24)>
 MPL: claim 3
 NTE: or pharmaceutically acceptable salts or esters
 NTE: oxo substitution also claimed
 NTE: also incorporates broader disclosure

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

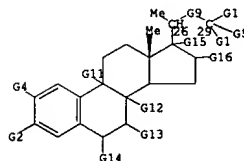
L9 ANSWER 8 OF 14 MARPAT COPYRIGHT 2003 ACS ON STN
 ACCESSION NUMBER: 133:350395 MARPAT
 TITLE: Synthesis of cholestane compounds with a C17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy
 INVENTOR(S): Hease, Robert Henry; Setty, Sundara Katugam; Srinivasasetty; Ramgopal, Malathi; Kugabalu-sooriar, Sanga
 PATENT ASSIGNEE(S): Marsden, John, Christopher, UK; Research Institute for Medicine and Chemistry Inc.
 SOURCE: PCT Int. Appl., 75 pp.
 CODEN: PIKX02
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000068246	A1	20001116	WO 2000-GB1813	20000511
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, FR, GB, GD, GE, GH, GM, GR, GU, HU, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1179005	A1	20020213	EP 2000-927569	20000511
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
ZA 2001009272	A	20021128	ZA 2001-9272	20011109
NO 2001005520	A	20020109	NO 2001-5520	20011112
PRIORITY APPLN. INFO.:			GB 1999-10934	19990511
			WO 2000-GB1813	20000511

AB Synthesis of cholestane compds. (I) [R1 and R2, which may be the same or different, = alkyl, alkenyl, alkynyl; R3 = Me having .alpha.- or .beta.-configuration; R4 = H or an etherifying or esterifying group; R5 = H, OH, alkoxy; X = OR4, wherein R4 is as defined above, or NR6R7 wherein R6 = H, alph. or aralph. org. group, acyl group comprising aliph., aralph. or aryl org. group linked to the nitrogen atom by way of a carbonyl group; R7 = H, alkyl; Y = (un)substituted alkylene, alkenylene, alkynylene; dotted lines signify that double bonds may be present at the 16(17)-position and/or either at the 6(7)- and 8(9)-positions or at the 7(8)-position] is disclosed for modulation of cell growth and differentiation, while having low calcemic activity. Thus, I [R1,R2 = Me; R3 = .alpha.-Me; R4,R5 = H; X = NHAc; Y = (CH2)4; .DELTA.16 double bond] is prepd. by reaction of 3-triisopropylsilyloxy-19-norchole-1,3,5(10),16-tetraene-24-bromide with acetonitrile followed by reduct. of nitrile to amine, methylation of amine with Me lithium, acetylation of the amino with acetic anhydride and desilylation with TBAF.

MYST 1

L9 ANSWER 8 OF 14 MARPAT COPYRIGHT 2003 ACS ON STN (Continued)



G1 = loweralkyl
 G2 = OH
 G9 = loweralkylene (SO G10)
 G10 = OH
 MPL: claim 1

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 9 OF 14 MARPAT COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 132:152024 MARPAT
 TITLE: Preparation of steroids as inhibitors of type 3
 3.alpha.-hydroxysteroid dehydrogenase
 INVENTOR(S): Labrie, Fernand; Merand, Yves; Gauthier, Sylvain;
 Provencher, Louis; Luu-The, Van
 PATENT ASSIGNEE(S): Endorecherche, Inc., Can.
 SOURCE: PCT Int. Appl., 140 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000007576	A2	20000217	WO 1999-CA724	19990806
WO 2000007576	A3	20000330		
V: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1321146	A2	20030625	EP 2003-4941	19990310
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
CA 2339368	AA	20000217	CA 1999-2339368	19990806
AU 9951449	A1	20000228	AU 1999-51449	19990806
EP 1102592	A2	20010530	EP 1999-936218	19990806
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002522380	T2	20020723	JP 2000-563261	19990806
NO 2001000651	A	20010405	NO 2001-651	20010207

PRIORITY APPLN. INFO.:

AB Novel methods of treating and/or inhibiting development of prostatic cancer, benign prostatic hyperplasia, prostatitis, acne, seborrhea, hirsutism or androgenic alopecia utilize inhibitors of type 3 3.alpha.-hydroxysteroid dehydrogenase alone or in combination with other active pharmaceuticals such as inhibitors of type 5 17.beta.-hydroxysteroid dehydrogenase. The inhibitors, of formula I (R1 = OH, acyloxy, alkoxy, amido, etc.; R2, R4 = H, CH, F, Cl, Br, NO2; R3 = alkoxy, acyloxy, alkoxy, alkoxy, OH, carbamate; R5 = H, alkyl, etc.; R1R5 = O, lactone ring; R6, R7 = H, alkyl, benzyl; R6R7 = cycloalkene), are prepd. Thus, I showed 98% inhibition of the transformation of 4-dione by type 3 3.alpha.-HSD. Pharmaceutical compns. contg. I are described.

MSTR 1

L9 ANSWER 10 OF 14 MARPAT COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 131:89084 MARPAT
 TITLE: Preparation of novel antiestrogenic steroids
 INVENTOR(S): Tanabe, Masato; Peters, Richard H.; Chao, Wan-Rui;
 Jong, Ling
 PATENT ASSIGNEE(S): SRI International, USA
 SOURCE: PCT Int. Appl., 142 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 4
 PATENT INFORMATION:

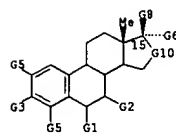
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9933859	A2	19990708	WO 1998-US27406	19981223
WO 9933859	A3	19991223		
V: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6054446	A	20000425	US 1997-998877	19971224
AU 9920104	A1	19990719	AU 1999-20104	19981223
AU 749597	B2	20020627		
EP 1056768	A2	20001206	EP 1998-964882	19981223
EP 1056768	B1	20030319		
R: DE, FR, GB, IT, NL				
JP 2001525855	T2	20011211	JP 1999-535172	19981223
EP 1310509	A2	20030514	EP 2003-183	19981223
R: DE, FR, GB, IT, NL				
NO 2000003254	A	20000821	NO 2000-3254	20000622

PRIORITY APPLN. INFO.:

AB Novel anti-estrogenic compds., e.g. I [X = hydrocarbyl including at least one O, N, S; X1 = H, hydrocarbyl including at least one O, N, S; XX1 = heterocycle; Y = C, N; R1 = H, alkyl, halo, alkylidene; R2, R3 = H, OH, alkyl, alkenyl, aryl, etc.; R4 = H, alkyl; R5 = H, alkoxy, halo, CN, CHO, etc.; R6 = H, alkyl, acyl, aryl, SO2NH2; R7 = H, halo, NO2, CHO, allyl, amino, etc.; R8 = H, OH, etc.; R9 = H, alkyl; R10 = Me, Et], are prepd. which are useful to treat a variety of disorders, particularly estrogen-dependent disorders. Preferred compds. have 1,3,5-estratriene nucleus, and are substituted at the C-17 or C-11 position with a mol. moiety which renders the compds. effective to competitively block the binding of estrogen to its receptor. Particularly preferred compds. are 17-deoxy-1,3,5-estratrienes. Thus, the citrate salt of II was prepd. and was shown to have antitumor activity against tamoxifen-resistant human mammary carcinoma at a dose of 25mg/kg/day.

MSTR 3

L9 ANSWER 9 OF 14 MARPAT COPYRIGHT 2003 ACS on STN (Continued)

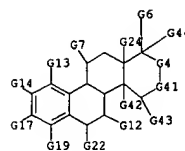


G3 = alkoxy<(1-20)>
 G6 = hydrocarbyl<(2-14)> (SO (1-1) G7)
 G7 = CO2H / alkoxy<(1-3)> / alkyl<(1-5)>
 G10 = 35



MPL: claim 3

L9 ANSWER 10 OF 14 MARPAT COPYRIGHT 2003 ACS on STN (Continued)



G3 = 23



G4 = 28



G17 = OH
 G24 = Me
 G25 = Ak (SR (1-) G26)
 G27 = O
 G31 = alkyl<(1-24)>
 DER: or pharmaceutically acceptable salts or esters
 DER: or pharmaceutically acceptable salts or esters
 MPL: claim 20
 NTE: oxo substitution also claimed

L9 ANSWER 11 OF 14 MARPAT COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 122:81747 MARPAT
 TITLE: Preparation of polyaminosteroids as bactericides and antifungals
 INVENTOR(S): Frye, Leah L.; Zasloff, Michael A.; Kinney, William A.; Moriarty, Robert M.
 PATENT ASSIGNEE(S): Magainin Pharmaceuticals Inc., USA
 SOURCE: PCT Int. Appl., 129 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 5
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9420520	A1	19940915	WO 1994-US2397	19940310
V: AU, CA, JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2157594	AA	19940915	CA 1994-2157594	19940310
AU 9463974	A1	19940926	AU 1994-63974	19940310
AU 692766	B2	19980618		
EP 688333	A1	19951227	EP 1994-911470	19940310
EP 688333	B1	19980819		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 08507527	T2	19960813	JP 1994-520212	19940310
AT 169930	E	19980915	AT 1994-911470	19940310
ES 2123133	T3	19990101	ES 1994-911470	19940310
US 5637691	A	19970610	US 1994-290826	19940818
CA 2185123	AA	19950914	CA 1994-2185123	19940913
WO 9524415	A1	19950914	WO 1994-US10265	19940913
V: AU, CA, JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9480101	A1	19950925	AU 1994-80101	19940913
AU 700344	B2	19981224		
EP 749437	A1	19961227	EP 1994-931274	19940913
EP 749437	B1	20011205		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 09509959	T2	19971007	JP 1994-523429	19940913
AT 210144	E	20011215	AT 1994-931274	19940913
ES 2164110	T3	20020216	ES 1994-931274	19940913
US 5721226	A	19980224	US 1995-478763	19950607
PRIORITY APPLN. INFO.:				
US 1993-29018 19930310				
WO 1994-US2397 19940310				
US 1994-290826 19940818				
WO 1994-US10265 19940913				
US 1995-416893 19950420				

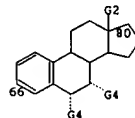
AB Title compds. (I) X = cationic hydrophilic side chain having .gtoreq.2 pos. charged amino groups; Y = anionic hydrophilic side chain; the steroid nucleus includes satd., unsatd., or partially satd. rings and .gtoreq.1 substituent selected from OH, SH, F, alkyl, alkoxy, amino; with the exception of squalamine) and related compds., were prep'd. Thus, 5.alpha.-cholestan-3-one was reductively aminated with BOC-NH(CH₂)₄N(BOC)(CH₂)₃NH₂ and NaBH₃CN in MeOH to give 71% of an .alpha.,.beta.-mixture of protected cholestan-3-amine which were deprotected with CF₃CO₂H in CHCl₃ to give title compd. II and the .beta.-isomer. II showed a min. inhibitory concn. of 2-4 .mu.g/mL against

L9 ANSWER 11 OF 14 MARPAT COPYRIGHT 2003 ACS on STN (Continued)
 Staphylococcus aureus, vs. 0.5-1 .mu.g/mL for squalamine.

MYR 1

G13-G1-G24

G1 = 66-1 80-3



G2 = alkyl<(1-4)>

G19 = O

G24 = 206



G25 = alkyl<(1-3)>

G26 = alkyl<(1-10)> (SR G27)

G27 = CO₂H / OH / CF₃

MPL: claim 1

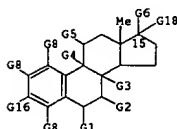
NTE: substitution is restricted

L9 ANSWER 12 OF 14 MARPAT COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 114:43309 MARPAT
 TITLE: Preparation of sulfonic acid-substituted aromatic steroids as inhibitors of steroid 5.alpha.-reductase
 INVENTOR(S): Holt, Dennis Alan; Metcalf, Brian Walter; Levy, Mark Alan
 PATENT ASSIGNEE(S): SmithKline Beecham Corp., USA
 SOURCE: Eur. Pat. Appl., 26 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 375347	A1	19900627	EP 1989-313260	19891219
EP 375347	B1	19941221		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 4970205	A	19901113	US 1988-290020	19881223
IL 91968	A1	19941021	IL 1989-91968	19891012
CN 1051181	A	19910508	CN 1989-108217	19891024
CA 2005215	AA	19900623	CA 1989-2005215	19891212
ZA 8909669	A	19901128	ZA 1989-9669	19891218
DK 8906451	A	19900624	DK 1989-6451	19891219
ES 2066003	T3	19950301	ES 1989-313260	19891219
AU 8947005	A1	19900628	AU 1989-47005	19891220
AU 627528	B2	19920827		
JP 02225494	A2	19900907	JP 1989-330927	19891220
AU 9229602	A1	19930121	AU 1992-29602	19921124
AU 655691	B2	19950105		
PRIORITY APPLN. INFO.:				
US 1988-290020 19881223				

AB Title steroids I (X₁, X₂, X₃ = H, Cl, F, Br, iodo, CF₃, alkyl, OH, alkoxy, CN, NO₂, N(R₁)₂, CO₂R₁, CHO; R = (1) .alpha.-H, .alpha.-OH, or .alpha.-OAc, and/or various carbonyl-contg. mono- or divalent radicals, (2) .beta.-acylamino, .beta.-cyano, or .beta.-tetrazolyl and .alpha.-H, (3) keto, etc.; R₁ = H, alkyl) and their salts were prep'd. For example, Me estrone underwent a sequence of conversion to its enol triflate, aminocarbonylation using (iso-Pr)₂NH, hydrogenation of .DELTA¹⁶, and demethylation of 3-OMe to give 3-hydroxyestr-1,3,5(10)-triene-17.beta.-(N,N-diisopropylcarboxamide). Acylation of 3-OH with Me₂NC(S)Cl, isomerization, and hydrolysis gave the 3-thiol, which was oxidized by O and KOH in DMF to give K estratriene-sulfonate deriv. II. The inhibition const. (K_i) of II for steroid 5.alpha.-reductase from hyperplastic human prostate was 10 nM. Ten I are claimed, and preps. with data are given for addnl. precursors of I.

MYR 2A



L9 ANSWER 13 OF 14 MARPAT COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 112:198890 MARPAT
 TITLE: Preparation of estratriene derivatives as steroid
 5.alpha.-reductase inhibitors
 INVENTOR(S): Holt, Dennis Alan; Levy, Mark Alan; Metcalf, Brian
 Walter
 PATENT ASSIGNEE(S): SmithKline Beckman Corp., USA
 SOURCE: Eur. Pat. Appl., 29 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

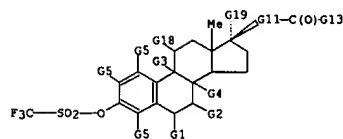
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 343954	A2	19891129	EP 1989-305246	19890524
EP 343954	A3	19900516		
EP 343954	B1	19941130		
WO 8911282	A1	19891130	WO 1989-US2269	19890523
W: AU, DK, JP				
AU 8937487	A1	19891212	AU 1989-37487	19890523
AU 627466	B2	19920827		
JP 03504498	T2	19911003	JP 1989-506391	19890523
CA 1331457	A1	19940816	CA 1989-600335	19890523
ES 2065378	T3	19950216	ES 1989-305246	19890524
ZA 8903971	A	19900530	ZA 1989-3971	19890525
US 4954446	A	19900904	US 1989-380226	19890714
IL 105198	A1	19940227	IL 1989-105198	19891012
DK 9002797	A	19901123	DK 1990-2797	19901123
DK 168295	B1	19940307		
DK 9301303	A	19931119	DK 1993-1303	19931119
DK 169787	B1	19950227		

PRIORITY APPLN. INFO.: US 1988-198534 19880525
 WO 1989-US2269 19890523

AB The title compds. (I; X1, X2, X3 = H, halo, CF3, Cl-6 alkyl, OH, etc.; A = O, S; R = O, 1; R1 = H, alkyl, R2 = mono- or divalent radical, e.g., H, alkyl, etc.) (II) useful as steroid 5.alpha.-reductase inhibitors, were prepd. E.g., 17.beta.-(diisopropylcarbamoyl) estr-1,3,5(10)-triene-3-carboxylic acid (II) was prepd. in many steps from estrone via trifluoromethylsulfonylation, carbamoylation, methoxycarbonylation, and hydrogenation. II in vitro inhibited human steroid 5.alpha.-reductase with a Ki of 19 nM. Tablets were formulated contg. I.

MPTR 27

L9 ANSWER 13 OF 14 MARPAT COPYRIGHT 2003 ACS on STN (Continued)



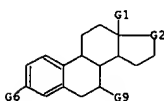
G11 = alkylene<(1-12)>
 G13 = alkyl<(1-8)> (SO (1-) OH)
 MPL: claim 15

L9 ANSWER 14 OF 14 MARPAT COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 110:115181 MARPAT
 TITLE: New 7-aryl-substituted 19-norsteroids useful as
 antiproliferatives, antiestrogens, and/or estrogens,
 and their preparation, use as medicines, and
 pharmaceutical compositions
 INVENTOR(S): Nique, Francois; Nedelec, Lucien; Bouton, Marie
 Madeleine; Philibert, Daniel
 PATENT ASSIGNEE(S): Roussel-Uclaf, Fr.
 SOURCE: Eur. Pat. Appl., 33 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 280618	A1	19880831	EP 1988-400371	19880218
EP 280618	B1	19920930		
FR 2610933	A1	19880819	FR 1987-2072	19870218
FR 2610933	B1	19890609		
ZA 8801030	A	19890426	ZA 1988-1030	19880215
FI 8800742	A	19880819	FI 1988-742	19880217
FI 92589	B	19940831		
AU 8811785	A1	19880825	AU 1988-11785	19880217
AU 610560	B2	19910523		
US 4874754	A	19891017	US 1988-157417	19880217
CA 1313653	A1	19930216	CA 1988-559130	19880217
FI 92589	C	19941212	FI 1988-742	19880217
JP 63222198	A2	19880916	JP 1988-34136	19880218
AT 81133	E	19921015	AT 1988-400371	19880218
ES 2043862	T3	19940101	ES 1988-400371	19880218
			FR 1987-2072	19870218
			EP 1988-400371	19880218

AB 19-Norsteroids I [A ring = A1, A2; R = Me, Et; R1 = acyl, alkoxyl, (un)protected OH; R2 = H, (un)substituted C.g.toreq.8 alkyl, alkenyl, or alkynyl, C.g.toreq.15 aryl or aralkyl; R1R2 = OCOCH2CH2, OCOCH:CH, O(CH2)3, OCH2CH:CH; Ar = (un)substituted 5- or 6-membered aryl] are prepd. for use as antiproliferatives, antiestrogens, and/or estrogens. A soln. of 4-BzMeCGH4OCH2CH2NMe2 in THF was treated with CuCl and then with 17.beta.-acetoxyestra-4,6-dien-3-one at -35.degree. to give I [A = A1, R = Me, R1 = OAc, R2 = H, Ar = alpha- and .beta.-C6H4OCH2CH2NMe2-4-.beta./alpha. > 2:1]. The 7.alpha.-isomer was aromatized by CuBr2 and LiBr at 75.degree. in MeCN, and saponid. by KOH in MeOH, to give [[(dimethylamino)ethoxy]phenyl]estratrienediol II. The concn. of II giving 50% inhibition of growth of mammary tumor cells MCF-7 in a fetal calf serum culture was 0.1 nM.

MPTR 18



L9 ANSWER 14 OF 14 MARPAT COPYRIGHT 2003 ACS on STN (Continued)

G1 = Me
 G2 = 21



G4 = Ak<(-8)> (SO (1-) G5)
 G5 = acyl / COpH / alkoxy carbonyl
 G6 = OH
 DER: and acid- and base-addition salts
 MPL: claim 1

=> d his

(FILE 'HOME' ENTERED AT 13:06:43 ON 07 OCT 2003)

FILE 'REGISTRY' ENTERED AT 13:06:52 ON 07 OCT 2003

L1 STRUCTURE UPLOADED

L2 6 S L1

L3 STRUCTURE UPLOADED

L4 5 S L3

L5 66 S L3 FULL

FILE 'CAPLUS' ENTERED AT 13:09:38 ON 07 OCT 2003

L6 3 S L5

FILE 'BEILSTEIN' ENTERED AT 13:13:14 ON 07 OCT 2003

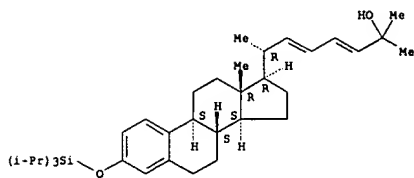
L7 4 S L5

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L8 15 S L5 FULL

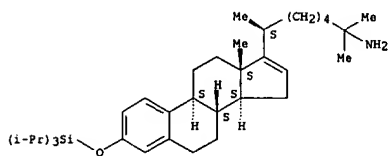
L9 14 S L8/COM

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



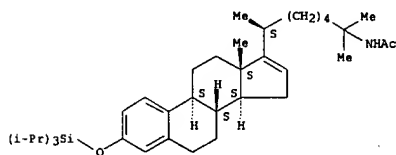
RN 305813-55-2 CAPLUS
CN 19-Norpregna-1,3,5(10),16-tetraene-20-pentanamine, .alpha.,.alpha.-dimethyl-3-[[[tris(1-methylethyl)silyl]oxy]-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305813-56-3 CAPLUS
CN Acetamide, N-[(6S)-1,1-dimethyl-6-[3-[[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10),16-tetraen-17-yl]heptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

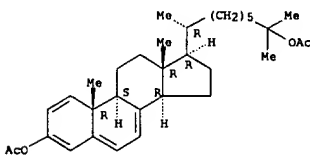


RN 305813-58-5 CAPLUS
CN 19-Norpregna-1,3,5(10),6,16-pentaene-20-pentanamine, .alpha.,.alpha.-dimethyl-3-[[[tris(1-methylethyl)silyl]oxy]-, (20R)- (9CI) (CA INDEX NAME)

L4 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

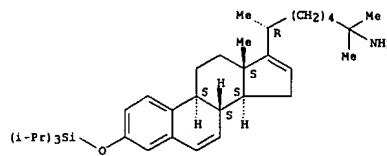
ACCESSION NUMBER: 1995:441032 CAPLUS
DOCUMENT NUMBER: 122:291299
TITLE: Synthesis of 24,24-dihomo-1.alpha.,25-dihydroxyvitamin D3
AUTHOR(S): Tachibana, Yoji
CORPORATE SOURCE: Res. Cent., Nisshin Flour Milling Co., Ltd., Saitama, 356, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1994), 42(11), 2349-51
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:291298
AB An alternative synthesis of 24,24-dihomo-1.alpha.,25-dihydroxyvitamin D3 was achieved starting from stigmastanol or cholenic acid.
IT 146310-89-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of dihomodihydroxyvitamin D3)
RN 146310-89-6 CAPLUS
CN Pregna-1,3,5,7-tetraene-20-hexanol, 3-(acetyloxy)-.alpha.,.alpha.-dimethyl-, acetate, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



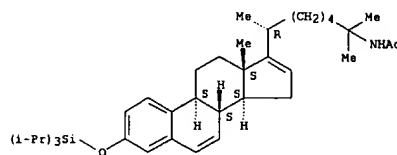
L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

Absolute stereochemistry.



RN 305813-59-6 CAPLUS
CN Acetamide, N-[(6R)-1,1-dimethyl-6-[3-[[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10),6,16-pentaen-17-yl]heptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

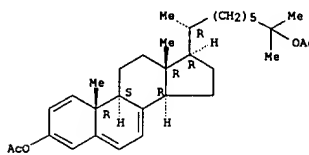


REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1993:124882 CAPLUS
DOCUMENT NUMBER: 118:124882
TITLE: Preparation of active vitamin D3 derivative as cell differentiation inducer
INVENTOR(S): Tachibana, Yoji
PATENT ASSIGNEE(S): Nisshin Flour Milling Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXKAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
PATENT NO. KIND DATE APPLICATION NO. DATE
JP 04300865 A2 19921023 JP 1991-89174 19910329
JP 3129758 B2 20010131
PRIORITY APPL. INFO.: JP 1991-89174 19910329
OTHER SOURCE(S): CASREACT 118:124882
AB 24,24-Dihomo-1.alpha.,25-dihydroxyvitamin D3 (II), showing cell differentiation activity (no data), is prepd. from 24,24-dihomocholesta-5,7-diene-1.alpha.,3.beta.,25-triol (I) by photoirradn. and subsequent thermal isomerization. A soln. of I (prepn. given) in Et2O-THF was irradiated by UV, concd., and then after addn. of EtOH, the soln. was heated under reflux for 1 h to give 24% II.
IT 146310-89-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and radn. of)
RN 146310-89-6 CAPLUS
CN Pregna-1,3,5,7-tetraene-20-hexanol, 3-(acetyloxy)-.alpha.,.alpha.-dimethyl-, acetate, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

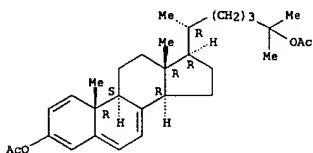


L4 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1992:6827 CAPLUS
 DOCUMENT NUMBER: 116:6827
 TITLE: Preparation of cholesta-5,7-diene-1.alpha.,3.beta.,25-triol as intermediate for 1.alpha.,25-dihydroxyvitamin D3
 INVENTOR(S): Tachibana, Yoji
 PATENT ASSIGNEE(S): Nisshin Flour Milling Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
 CODEN: JKKXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

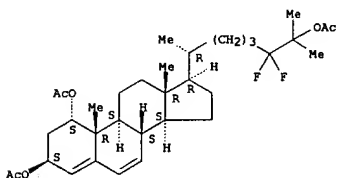
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03118392	A2	19910520	JP 1989-254837	19890929
JP 2953665	B2	19990927		

PRIORITY APPLN. INFO.: JP 1989-254837 19890929
 OTHER SOURCE(S): CASREACT 116:6827; MARPAT 116:6827
 AB The title compd. (I) is prep'd. via oxidn. of 25-hydroxycholesterol by DDQ, protection of 25-OH in resulting 25-hydroxy-cholesta-1,4,6-triene-3-one II (R = OH), reaction of II (X = protected OH) with AcOCMe:CH2 in the presence of acids, redn. of obtained acetate III, Diels-Alder reaction of alc. IV with 4-phenyl-1,2,4-triazoline-3,5-dione, protection of 3-OH in the adduct V, epoxidn. of 1,2-double bond, deprotection of 3-OH, and redn. of the resulting epoxide VI.
 IT 137342-87-19
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and redn. of)
 RN 137342-87-1 CAPLUS
 CN Cholesta-1,3,5,7-tetraene-3,25-diol, diacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



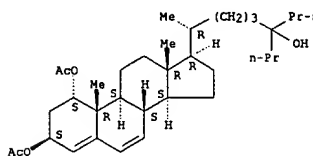
L4 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



L4 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1988:473745 CAPLUS
 DOCUMENT NUMBER: 109:73745
 TITLE: 26,27-Diethyl-1.alpha.,25-dihydroxyvitamin D3 and 24,24-difluoro-24-homo-1.alpha.,25-dihydroxyvitamin D3: highly potent inducer for differentiation of human leukemia cells HL-60
 AUTHOR(S): Ikekawa, Nobuo; Eguchi, Tadashi; Hara, Noriyuki; Takatsuto, Suguru; Honda, Atsushi; Mori, Yo; Otomo, Susumu
 CORPORATE SOURCE: Dep. Chem., Tokyo Inst. Technol., Tokyo, 152, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (1987), 35(10), 4362-5
 CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 109:73745
 AB 26,27-Diethyl-1.alpha.,25-dihydroxyvitamin D3 (I) and 24,24-difluoro-24-homo-1.alpha.,25-dihydroxyvitamin D3 (II) were synthesized. They had almost no vitamin D activity but were more active than 1.alpha.,25-dihydroxyvitamin D3 in tests for induction of cell differentiation.
 IT 115540-34-6P 115540-40-4P
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, during synthesis of vitamin D3 analogs)
 RN 115540-34-6 CAPLUS
 CN Pregna-4,6-diene-1,3-diol, 20-(4-hydroxy-4-propylheptyl)-, 1,3-diacetate, (1.alpha.,3.beta.,20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

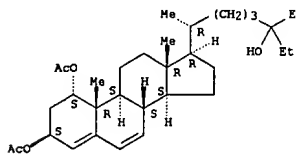


RN 115540-40-4 CAPLUS
 CN Pregna-4,6-diene-1,3-diol, 20-[5-(acetyloxy)-4,4-difluoro-5-methylhexyl]-, diacetate, (1.alpha.,3.beta.,20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

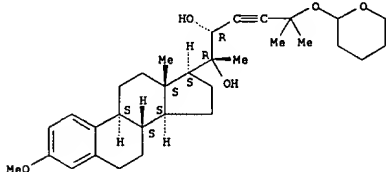
L4 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1985:471584 CAPLUS
 DOCUMENT NUMBER: 103:71584
 TITLE: Synthesis of 1.alpha.,25-dihydroxy-26,27-dimethylvitamin D3, a highly active analog of 1.alpha.,25-dihydroxyvitamin D3
 AUTHOR(S): Sai, Hiroshi; Takatsuto, Suguru; Hara, Noriyuki; Ikekawa, Nobuo
 CORPORATE SOURCE: Dep. Chem., Tokyo Inst. Technol., Tokyo, 152, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (1985), 33(2), 878-81
 CODEN: CPBTAL; ISSN: 0009-2363
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 103:71584
 AB Title vitamin D3 deriv. I was prep'd. from epoxy(tetrahydropyranyloxy)dinor choleladienone II and was more active than 1.alpha.,25-dihydroxyvitamin D3. Key transformations in the prepn. of I included Wittig condensation of norcholeladienone III (R = MeOCH2) with Ph3P:CHCO2Et and subsequent hydrogenation, Grignard reaction with EtBr, and hydrolysis to give the tertiary alc. IV (R = H).
 IT 97453-13-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and sapon. of)
 RN 97453-13-9 CAPLUS
 CN Pregna-4,6-diene-1,3-diol, 20-(4-ethyl-4-hydroxyhexyl)-, 1,3-diacetate, (1.alpha.,3.beta.,20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2003 ACS ON STN
 ACCESSION NUMBER: 1985:471583 CAPLUS
 DOCUMENT NUMBER: 103:71583
 TITLE: A stereoselective synthesis of 1,2-diols from .alpha.-hydroxyaldehydes
 AUTHOR(S): Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.; Horn, Dennis H. S.
 CORPORATE SOURCE: Dep. Chem., Univ. Wyoming, Laramie, WY, 82071, USA
 SOURCE: Tetrahedron Letters (1985), 26(9), 1189-92
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 103:71583
 AB The addn. of LiC.tplbond.CMe2O-THP (THP = tetrahydro-2H-pyran-2-yl) to (20R)-20-hydroxypregnane-20-carboxaldehydes I and II in the absence and in the presence of BF3 afforded predominantly 20R,22R-diols III and IV or 20R,22S-diols V and VI, resp., characteristic of ecdysones.
 IT 97452-83-0P 97452-84-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and hydrolysis-hydrogenation of)
 RN 97452-83-0 CAPLUS
 CN 19-Norcholesta-1,3,5(10)-trien-23-yne-20,22-diol, 3-methoxy-25-[(tetrahydro-2H-pyran-2-yl)oxy]-, (22R)- (9CI) (CA INDEX NAME)

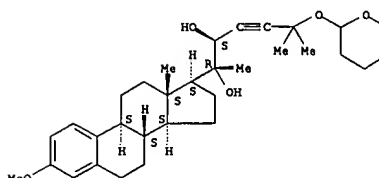
Absolute stereochemistry.



RN 97452-84-1 CAPLUS
 CN 19-Norcholesta-1,3,5(10)-trien-23-yne-20,22-diol, 3-methoxy-25-[(tetrahydro-2H-pyran-2-yl)oxy]-, (22S)- (9CI) (CA INDEX NAME)

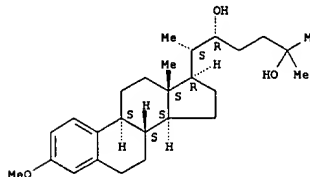
Absolute stereochemistry.

L4 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2003 ACS ON STN (Continued)



IT 97452-85-2P 97452-86-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 97452-85-2 CAPLUS
 CN 19-Norcholesta-1,3,5(10)-trien-22,25-diol, 3-methoxy-, (22R)- (9CI) (CA INDEX NAME)

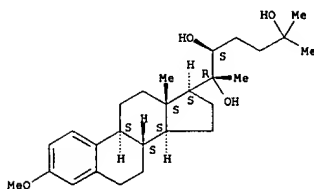
Absolute stereochemistry.



RN 97452-86-3 CAPLUS
 CN 19-Norcholesta-1,3,5(10)-trien-20,22,25-triol, 3-methoxy-, (22S)- (9CI) (CA INDEX NAME)

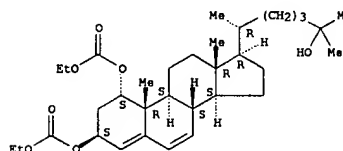
Absolute stereochemistry.

L4 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2003 ACS ON STN (Continued)



L4 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2003 ACS ON STN
 ACCESSION NUMBER: 1985:62515 CAPLUS
 DOCUMENT NUMBER: 102:62515
 TITLE: An improved synthesis of 1.alpha.-hydroxy-7-dehydrocholesterol derivatives
 AUTHOR(S): Nishikawa, Osamu; Oshida, Junichi; Tsuruta, Hideki
 CORPORATE SOURCE: Pharm. Dev. Sect., Teijin Ltd., Iwakuni, 740, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (1984), 32(8), 3244-7
 CODEN: CPBTAL; ISSN: 0009-2363
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The effect of protective groups on the allylic bromination and the subsequent dehydrobromination of cholesterol and 1.alpha.-hydroxycholesterol derivs. I (R = Ac, Me3CCO, Me(CH2)4CO, EtO2C, PhCH2O2C; R1 = H, AcO, Me3CCO2, Me(CH2)4CO2, PhCH2O2CO, EtO2CO; R2 = H, (R)-EtO2CO; R3 = H, HO) was examd. 1.alpha.-Hydroxy-7-dehydrocholesterol derivs. were selectively obtained in high yield by using alkoxycarbonyl groups as protective groups.
 IT 79488-37-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, by bromination-dehydrobromination of cholesterol deriv.)
 RN 79488-37-2 CAPLUS
 CN Cholesta-4,6-diene-1,3,25-triol, 1,3-bis(ethyl carbonate), (1.alpha.,3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1984:22905 CAPLUS
 DOCUMENT NUMBER: 100:22905
 TITLE: Cholecalciferol derivatives
 INVENTOR(S): Barner, Richard; Hubscher, Josef
 PATENT ASSIGNEE(S): Hoffmann-La Roche, F. und Co. A.-G., USA
 SOURCE: U.S., 7 pp. Cont.-in-part of U.S. Ser. No. 333,354, abandoned.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4407754	A	19831004	US 1982-357438	19820312
CH 644100	A	19840713	CH 1979-8346	19790914
GB 2114569	A1	19830824	GB 1983-4071	19830214
GB 2114569	B2	19840523		

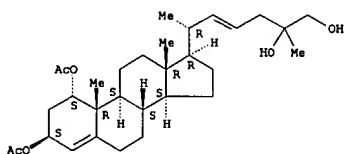
PRIORITY APPLN. INFO.: CH 1979-8346 19790914
 US 1980-183140 19800902
 US 1981-333354 19811222
 GB 1980-29544 19800912

AB Trihydroxycholecalciferol I was prepd. from pregnenecarboxaldehyde II (R,R1 = alkyl, acyl) via Wittig condensation with dioxolanylethylphosphonium salts III (R2, R3 = alkyl; R4 = aryl). Isomerizing I gave 1.alpha.,25,26-trihydroxycholecalciferol, useful for regulating Ca metab. or Ca transport in mammals (no data).

IT 88257-25-49
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and hydrogenation of)

RN 88257-25-4 CAPLUS
 CN Cholesta-4,22-diene-1,3,25,26-tetrol, 1,3-diacetate, (1.alpha.,3.beta.)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.



IT 88257-30-19
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and ring cleavage of)

L4 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1982:6958 CAPLUS
 DOCUMENT NUMBER: 96:6958
 TITLE: 1.alpha.-Hydroxy-7-dehydro steroids
 INVENTOR(S): Klausmeier, William H.; Johnson, Richard L.; Hirsch, Arnold L.
 PATENT ASSIGNEE(S): Diamond Shamrock Corp., USA
 SOURCE: U.S., 9 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4287129	A	19810901	US 1980-172925	19800728
EP 45884	A1	19820217	EP 1981-105846	19810723

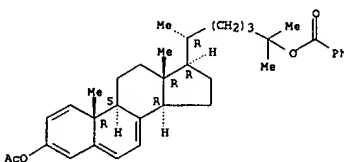
PRIORITY APPLN. INFO.: US 1980-172925 19800728

AB Unsatd. steroids I (R = cholestane side-chain substituted by HO, Aco, cholane side-chain substituted by Aco; R = alkyl) were prepd. as intermediates in the prepn. of vitamin D3 deriva. Thus, oxidn. of 25-hydroxycholesterol by dichlorodicyanobenzoquinone gave 58 25-hydroxycholesta-1,4,6-trien-3-one, which underwent benzoylation and then enolization-acetylation by treatment with Ac2O-AcCl in the presence of pyridine to give 3-acetoxy-25-benzoyloxycholesta-1,3,5,7-tetraene. The latter underwent successive Diels-Alder reaction with 4-phenyl-1,2,4-triazoline-3,5-dione, silylation, and epoxidn. to give epoxycholestaene adduct II, which underwent desilylation and LiAlH4 redn. to give 1.alpha.,25-dihydroxy-7-dehydrocholesterol.

IT 80097-53-69
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and redn. of)

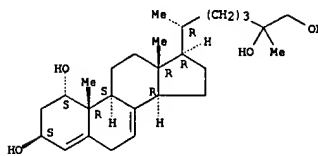
RN 80097-53-6 CAPLUS
 CN Cholesta-1,3,5,7-tetraene-3,25-diol, 3-acetate 25-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 RN 88257-30-1 CAPLUS
 CN Cholesta-4,7-diene-1,3,25,26-tetrol, (1.alpha.,3.beta.)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1981:56904 CAPLUS
 DOCUMENT NUMBER: 95:169604
 TITLE: Active-type vitamin D3 compounds and the cholesta-5,7-diene precursors
 INVENTOR(S): Nishikawa, Osamu; Ishimaru, Kenji; Takeshita, Toru; Tsuruta, Hideki
 PATENT ASSIGNEE(S): Teijin Ltd., Japan
 SOURCE: Eur. Pat. Appl., 53 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 28484	A1	19810513	EP 1980-303732	19801022
EP 28484	B1	19850814		
R: CH, DE, FR, GB, IT, NL, SE				
JP 56059737	A2	19810523	JP 1979-135871	19791023
JP 61045999	B4	19861011		
JP 56092267	A2	19810725	JP 1979-169464	19791227
JP 60034948	B4	19850812		
JP 56092268	A2	19810725	JP 1979-169465	19791227
JP 62051266	B4	19871029		
JP 56147765	A2	19811116	JP 1980-50258	19800418
JP 60034949	B4	19850812		
DK 8004473	A	19810424	DK 1980-4473	19801022
DK 160817	B	19910422		
DK 160817	C	19911007		
CA 1160217	A1	19840110	CA 1980-362937	19801022
US 4388243	A	19830614	US 1982-371870	19820426

PRIORITY APPLN. INFO.: JP 1979-135871 19791023
 JP 1979-169464 19791227
 JP 1979-169465 19791227
 JP 1980-50258 19800418
 US 1980-199126 19801022

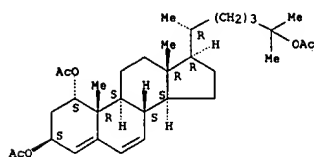
AB Cholestadienes I (R, R1 = alkoxy-carbonyl; R2 = H, alkoxy-carbonyloxy, R3 = H, alkoxy-carbonyloxy, HO) were prepd. as intermediates in the prepn. of 1.alpha.-hydroxycholecalciferol. Thus, treatment of 1.alpha.-hydroxycholesterol with ClCO2Et in CH2Cl2 contg. 4-(dimethylamino)pyridine gave 1.alpha.,3.beta.-bis(ethoxycarbonyloxy)cholesta-5-ene, which underwent photochem. bromination by dibromodimethylhydantoin in hexane and then dehydrobromination in xylene contg. collidine at 170.degree. to give I (R = R1 = EtO2C; R2 = R3 = H).

IT 61319-29-7P 79488-37-2P
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 61319-29-7 CAPLUS
 CN Cholesta-4,6-diene-1,3,25-triol, triacetate, (1.alpha.,3.beta.)-(9CI) (CA INDEX NAME)

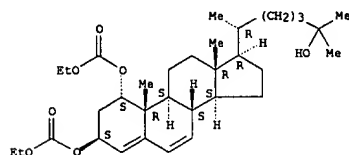
Absolute stereochemistry.

L4 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



RN 79488-37-2 CAPLUS
 CN Cholesta-4,6-diene-1,3,25-triol, 1,3-bis(ethyl carbonate),
 (1.alpha.,3.beta.)- (9CI) (CA INDEX NAME)

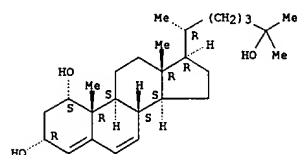
Absolute stereochemistry.



L4 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 67804-88-0 CAPLUS
 CN Cholesta-4,6-diene-1,3,25-triol, (1.alpha.,3.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



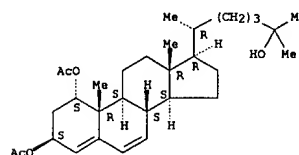
L4 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1978:559766 CAPLUS
 DOCUMENT NUMBER: 89:159786
 TITLE: Determination of 1.alpha.,25-dihydroxycholecalciferol
 INVENTOR(S): Baggiolini, Enrico; Uskokovic, Milan Radoje; Fairney, Angela
 PATENT ASSIGNEE(S): Hoffmann-La Roche, F. und Co. A.-G., Fed. Rep. Ger.
 SOURCE: Ger. Offen., 32 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2800782	A1	19780713	DE 1978-2800782	19780109
GB 1592170	A	19810701	GB 1977-538	19770107
DK 7800078	A	19780708	DK 1978-78	19780106
NL 7800224	A	19780711	NL 1978-224	19780106
JP 53087344	A2	19780801	JP 1978-314	19780106
FR 2376863	A1	19780804	FR 1978-414	19780109
FR 2376863	B1	19800801		
DK 8001254	A	19800321	DK 1980-1254	19800321

PRIORITY APPLN. INFO.: GB 1977-538 19770107
 DK 1978-78 19780106
 AB Antigens and antisera are prepd. and a radioimmunoassay (RIA) is described for detn. of 1.alpha.,25-dihydroxycholecalciferol (I) and its optical enantiomers and racemates. As antigen, 1.alpha.,25-dihydroxycholecalciferol 25-hemisuccinate (II), which was prepd. by a series of reactions starting with I, was coupled to bovine serum albumin. The II-serum albumin conjugate, in complete Freund's adjuvant, was injected into rabbits to elicit antibody prodn. I in human blood serum then was detd. by RIA that uses the anti-conjugate antiserum, I-3H as tracer, and dextran-coated charcoal to sep. free from bound antigen. The RIA is sensitive to pg amts. of I.
 IT (prepn. of, dihydroxycholecalciferol radioimmunoassay in relation to)
 RN 67804-87-9 CAPLUS
 CN Cholesta-4,6-diene-1,3,25-triol, 1,3-diacetate, (1.alpha.,3.beta.)- (9CI) (CA INDEX NAME)

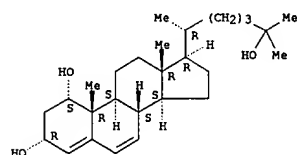
Absolute stereochemistry.



L4 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 67804-88-0 CAPLUS
 CN Cholesta-4,6-diene-1,3,25-triol, (1.alpha.,3.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

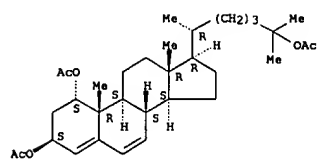
ACCESSION NUMBER: 1977:16846 CAPLUS
 DOCUMENT NUMBER: 86:16846
 TITLE: 1.alpha.,25-Dihydroxycholecalciferol
 INVENTOR(S): Uskokovic, Milan R.; Narwid, Thomas A.; Iacobelli, Jerome A.; Baggiolini, Enrico
 PATENT ASSIGNEE(S): Hoffmann-La Roche, F., und Co., A.-G., Switz.
 SOURCE: Ger. Offen., 25 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2607322	A1	19760902	DE 1976-2607322	19760223
DE 2607322	C2	19830601		
US 3993675	A	19761123	US 1975-552027	19750224
CH 622533	A	19810415	CH 1976-1173	19760130
JP 51108050	A2	19760925	JP 1976-17160	19760220
JP 59001278	B4	19840111		
BE 838823	A1	19760823	BE 1976-164533	19760223
FR 2301503	A1	19760917	FR 1976-4939	19760223
FR 2301503	B1	19800229		
GB 1539061	A	19790124	GB 1976-7028	19760223
GB 1539062	A	19790124	GB 1976-41939	19760223
AT 351187	B	19790710	AT 1976-1267	19760223
AT 7601267	A	19781215		
NL 7601872	A	19760826	NL 1976-1872	19760224
NL 173172	B	19830718		
NL 173172	C	19831216		
JP 58116457	A2	19830711	JP 1982-215630	19821210
JP 59012666	B4	19840324		

PRIORITY APPLN. INFO.: US 1975-552027 19750224
 GB 1976-7028 19760223
 AB 1.alpha.,25-Dihydroxycholecalciferol (I, R = H) was prepd. by irradiation of 3.beta.-hydroxy-1.alpha.,25-diacetoxycholesta-5,7-diene (II), sapon. of precholecalciferol III (R = Ac), and isomerization of III (R = H). Bromination-dehydrobromination of 1.alpha.,25-diacetoxycholesteryl acetate followed by sapon. gave II.
 IT 61319-29-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and hydrolysis-dehydration of)
 RN 61319-29-7 CAPLUS
 CN Cholesta-4,6-diene-1,3,25-triol, triacetate, (1.alpha.,3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



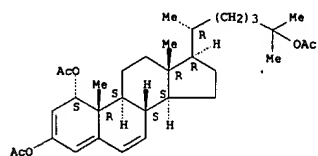
IT 61319-30-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 61319-30-0 CAPLUS

61519-30-0 CAPLOS
CN Cholesta-2,4,6-triene-1,3,25-triol, triacetate, (1.alpha.)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.



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(FILE 'HOME' ENTERED AT 07:50:11 ON 08 OCT 2003)

FILE 'REGISTRY' ENTERED AT 07:50:58 ON 08 OCT 2003

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 83 S L1 FULL

FILE 'CAPLUS' ENTERED AT 07:53:38 ON 08 OCT 2003

L4 14 S L3

L5 14 S L3/PREP

L6 0 S L5 NOT L4

09/926,491

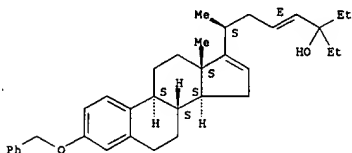
Page 1

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L4 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2003:263913 CAPLUS
 DOCUMENT NUMBER: 139:7056
 TITLE: Regio- and Stereoselective Ruthenium-Catalyzed Hydrovinylation of 1,3-Dienes: Application to the Generation of a 20(S) Steroidal Side Chain
 AUTHOR(S): He, Zhengjie; Yi, Chae S.; Donaldson, William A.
 CORPORATE SOURCE: Department of Chemistry, Marquette University, Milwaukee, WI, 53201-1881, USA
 SOURCE: Organic Letters (2003), 5(9), 1567-1569
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 139:7056
 AB The addn. of ethylene to 1,3-dienes and 1-vinylcycloalkenes, catalyzed by two ruthenium complexes, proceeds in a regioselective fashion to afford 3-methyl-1,4-dienes as products. For example, cyclohexene I (R = H, CMe=CH₂, R₁ = CH=CH₂) gives I (R₁ = CHMeCH=CH₂) in 57-62% yield. For a steroidal-based 1-vinylcycloalkene II, the addn. is stereospecific, giving a product with a 20(S) configuration.
 IT 539925-77-8P
 RL: SPN (Synthetic preparation); PREP (Preparation) (regio- and stereoselective ruthenium-catalyzed hydrovinylation of 1,3-dienes, vinylcycloalkenes, and steroidal diene)
 RN 539925-77-8 CAPLUS
 CN 4-Octen-3-ol, 3-ethyl-7-[3-(phenylmethoxy)estra-1,3,5(10),16-tetraen-17-yl]-, (4E,7S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
 Double bond geometry as shown.



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

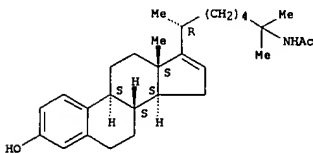
ACCESSION NUMBER: 2000:814500 CAPLUS
 DOCUMENT NUMBER: 133:350395
 TITLE: Synthesis of cholestane compounds with a C17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy
 INVENTOR(S): Hesse, Robert Henry; Setty, Sundara Katugam Srinivasasetty; Ramgopal, Malathi; Kugabalusooriar, Sanga
 PATENT ASSIGNEE(S): Marsden, John, Christopher, UK; Research Institute for Medicine and Chemistry Inc.
 SOURCE: PCI Int. Appl., 75 pp.
 CODEN: PIXX02
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000068246	A1	20001116	WO 2000-GB1813	20000511
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, FR, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RU, RO, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1179005	A1	20020213	EP 2000-927569	20000511
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
ZA 2001009272	A	20021128	ZA 2001-9272	20011109
NO 2001005520	A	20020109	NO 2001-5520	20011112
PRIORITY APPL. INFO.: GB 1999-10934 A 19990511 WO 2000-GB1813 W 20000511				

OTHER SOURCE(S): MARPAT 133:350395
 AB Synthesis of cholestane compds. (I) [R₁ and R₂, which may be the same or different, = alkyl, alkenyl, alkynyl; R₃ = Me having .alpha.- or .beta.-configuration; R₄ = H or an etherifying or esterifying group; R₅ = H, OH, alkoxy; X = OR₄, wherein R₄ is as defined above, or NR₆R₇ wherein R₆ = H, aliph. or araliph. org. group, acyl group comprising aliph., araliph. or acyl org. group linked to the nitrogen atom by way of a carbonyl group; R₇ = H, alkyl; Y = (un)substituted alkylene, alkenylene, alkynylene; dotted lines signify that double bonds may be present at the 16(17)-position and/or either at the 6(7)- and 8(9)-positions or at the 7(8)-position] is disclosed for modulation of cell growth and differentiation, while having low calcemic activity. Thus, I [R₁, R₂ = Me; R₃ = .alpha.-Me; R₄, R₅ = H; X = NHAc; Y = (CH₂)₄; .DELTA.16 double bond] is prep. by reaction of 3-triisopropylsilyloxy-19-norchole-1,3,5(10),16-tetraene-24-bromide with acetonitrile followed by redn. of nitrile to amine, methylation of amine with Me lithium, acetylation of the amino with acetic anhydride and desilylation with TBAF.
 IT 305812-17-3P 305812-18-4P 305812-19-5P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological

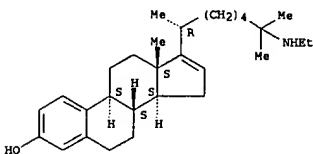
L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (synthesis of cholestane compds. with a C17-alkyl side chain and an arom. A-ring for use in cell modulating therapy)
 RN 305812-17-3 CAPLUS
 CN Acetamide, N-[(6R)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-18-4 CAPLUS
 CN 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-[5-(ethylamino)-5-methylhexyl]-, (20R)- (9CI) (CA INDEX NAME)

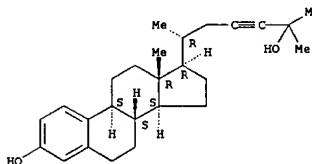
Absolute stereochemistry.



RN 305812-52-6 CAPLUS
 CN 19-Norcholesta-1,3,5(10)-trien-23-yne-3,25-diol (9CI) (CA INDEX NAME)

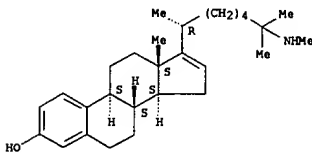
Absolute stereochemistry.

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



IT 305812-19-5P 305812-20-8P 305812-21-9P
 305812-22-0P 305812-23-1P 305812-24-2P
 305812-25-3P 305812-26-4P 305812-27-5P
 305812-28-6P 305812-29-7P 305812-30-0P
 305812-31-1P 305812-32-2P 305812-33-3P
 305812-34-4P 305812-35-5P 305812-36-6P
 305812-37-7P 305812-38-8P 305812-39-9P
 305812-40-2P 305812-41-3P 305812-42-4P
 305812-43-5P 305812-44-6P 305812-45-7P
 305812-46-8P 305812-47-9P 305812-48-0P
 305812-49-1P 305812-50-4P 305812-51-5P
 305812-52-6P 305812-53-7P 305812-54-8P
 305812-55-9P 305812-56-0P 305812-57-1P 305812-58-2P
 305812-59-3P 305812-60-6P 305812-61-7P
 305812-62-8P 305812-63-9P 305812-64-0P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (synthesis of cholestane compds. with a C17-alkyl side chain and an arom. A-ring for use in cell modulating therapy)
 RN 305812-19-5 CAPLUS
 CN 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-[5-methyl-5-(methylamino)hexyl]-, (20R)- (9CI) (CA INDEX NAME)

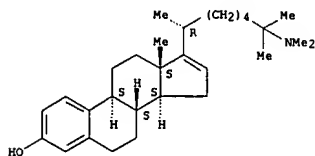
Absolute stereochemistry.



RN 305812-20-8 CAPLUS
 CN 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-[5-(dimethylamino)-5-methylhexyl]-, (20R)- (9CI) (CA INDEX NAME)

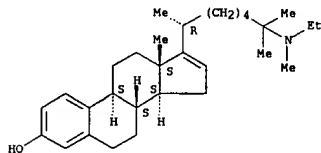
Absolute stereochemistry.

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



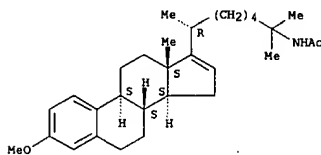
RN 305812-21-9 CAPLUS
CN 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-[(5-ethylmethylamino)-5-methylhexyl]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-22-0 CAPLUS
CN Acetamide, N-[(6R)-6-(3-methoxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

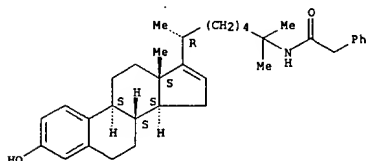


RN 305812-23-1 CAPLUS
CN Acetamide, N-[(6R)-6-(3-ethoxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

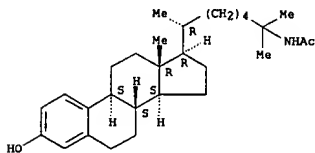
L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

Absolute stereochemistry.



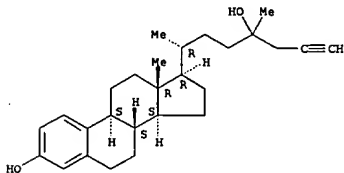
RN 305812-27-5 CAPLUS
CN Acetamide, N-[(6R)-6-[(17.beta.)-3-hydroxyestra-1,3,5(10)-trien-17-yl]-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



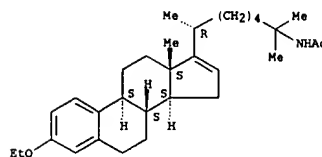
RN 305812-28-6 CAPLUS
CN 19,26,27-Trinorcholesta-1,3,5(10)-triene-3,24-diol, 24-(2-propynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



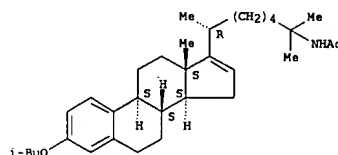
RN 305812-29-7 CAPLUS
CN 19,26,27-Trinorcholesta-1,3,5(10)-triene-3,24-diol, 2-methoxy-24-(2-propynyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



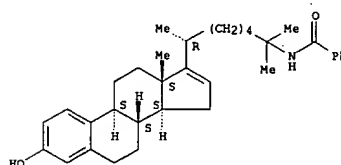
RN 305812-24-2 CAPLUS
CN Acetamide, N-[(6R)-1,1-dimethyl-6-[3-(2-methylpropoxy)estra-1,3,5(10),16-tetraen-17-yl]heptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-25-3 CAPLUS
CN Benzamide, N-[(6R)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

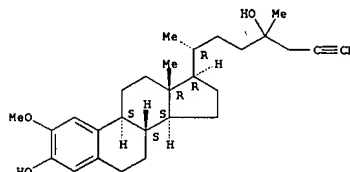
Absolute stereochemistry.



RN 305812-26-4 CAPLUS
CN Benzeneacetamide, N-[(6R)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

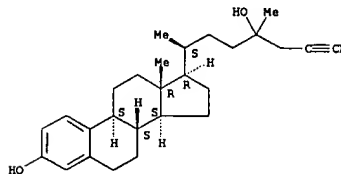
L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

Absolute stereochemistry.

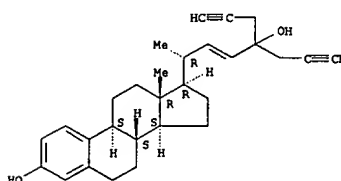


RN 305812-30-0 CAPLUS
CN 19,26,27-Trinorcholesta-1,3,5(10)-triene-3,24-diol, 24-(2-propynyl)-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



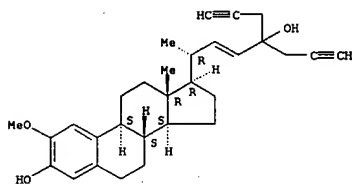
RN 305812-31-1 CAPLUS
CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-[3-hydroxy-3-(2-propynyl)-1-hexen-5-ynyl]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

RN 305812-32-2 CAPLUS
CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-[3-hydroxy-3-(2-propynyl)-1-hexen-5-ynyl]-, (20R)- (9CI) (CA INDEX NAME)

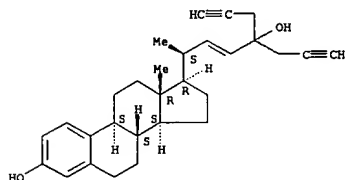
L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 ynyl]-2-methoxy-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.



RN 305812-33-3 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-[3-hydroxy-3-(2-propynyl)-1-hexen-5-ynyl]-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.

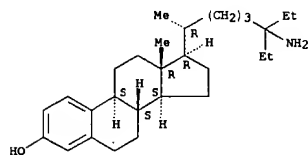


RN 305812-34-4 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethyl-2-hexynyl)-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

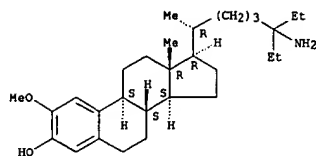
L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethylhexyl)-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



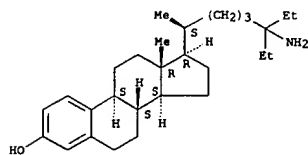
RN 305812-38-8 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethylhexyl)-2-methoxy-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



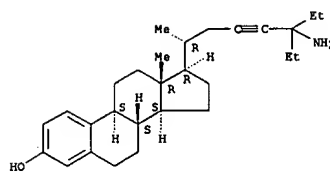
RN 305812-39-9 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethylhexyl)-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



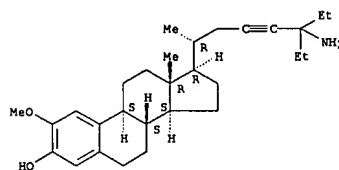
RN 305812-40-2 CAPLUS
 CN Acetamide, N-[(5R)-1,1-diethyl-5-[(17.beta.)-3-hydroxyestra-1,3,5(10)-trien-17-yl]-2-hexynyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



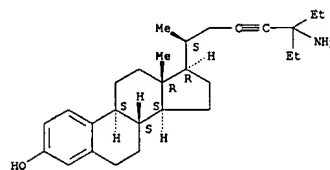
RN 305812-35-5 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethyl-2-hexynyl)-2-methoxy-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



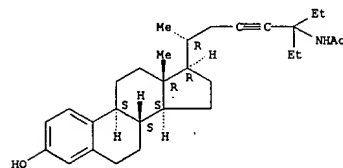
RN 305812-36-6 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethyl-2-hexynyl)-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



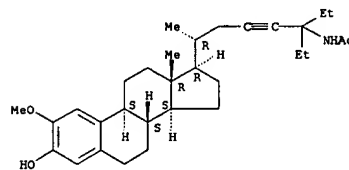
RN 305812-37-7 CAPLUS

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 Absolute stereochemistry.



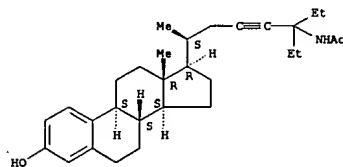
RN 305812-41-3 CAPLUS
 CN Acetamide, N-[(5R)-1,1-diethyl-5-[(17.beta.)-3-hydroxy-2-methoxyestra-1,3,5(10)-trien-17-yl]-2-hexynyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



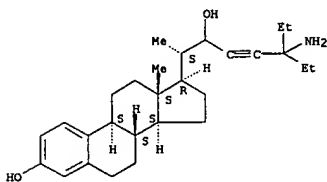
RN 305812-42-4 CAPLUS
 CN Acetamide, N-[(5S)-1,1-diethyl-5-[(17.beta.)-3-hydroxyestra-1,3,5(10)-trien-17-yl]-2-hexynyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



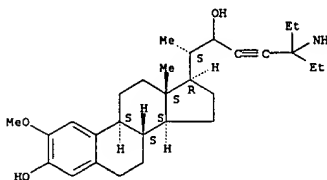
RN 305812-43-5 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentynyl)-3-hydroxy-, (20S)- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
Absolute stereochemistry.



RN 305812-44-6 CAPLUS
CN 19-Norpregna-1,3,5(10)-triene-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentynyl)-3-hydroxy-2-methoxy-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

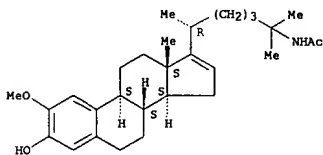


RN 305812-45-7 CAPLUS
CN 19-Norpregna-1,3,5(10)-triene-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentynyl)-3-hydroxy-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

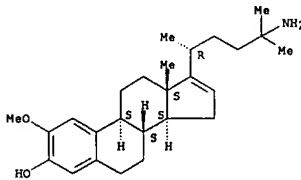
L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



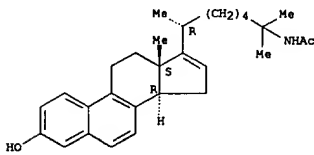
RN 305812-49-1 CAPLUS
CN 19,26,27-Trinorergosta-1,3,5(10),16-tetraen-3-ol, 24-amino-2-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



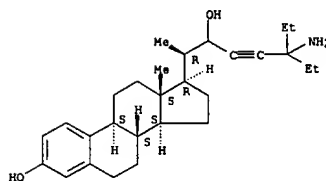
RN 305812-50-4 CAPLUS
CN Acetamide, N-[(6R)-6-(3-hydroxyestra-1,3,5,7,9,16-hexaen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



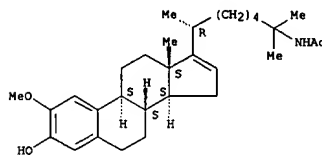
RN 305812-51-5 CAPLUS
CN 19-Norpregna-1,3,5,7,9,16-hexaen-3-ol, 20-(5-amino-5-methylhexyl)-, (20R)- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



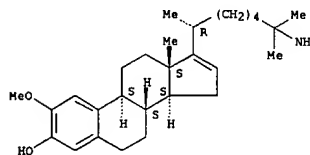
RN 305812-46-8 CAPLUS
CN Acetamide, N-[(6R)-6-(3-hydroxy-2-methoxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-47-9 CAPLUS
CN 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-(5-amino-5-methylhexyl)-2-methoxy-, (20R)- (9CI) (CA INDEX NAME)

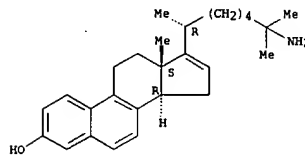
Absolute stereochemistry.



RN 305812-48-0 CAPLUS
CN Acetamide, N-(3-hydroxy-2-methoxy-19-norcholesta-1,3,5(10),16-tetraen-25-

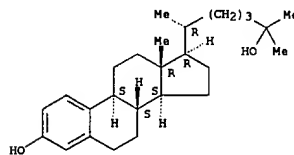
L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

Absolute stereochemistry.



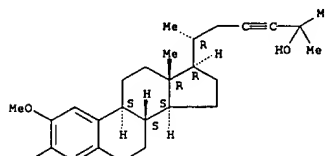
RN 305812-53-7 CAPLUS
CN 19-Norcholesta-1,3,5(10)-triene-3,25-diol (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-54-8 CAPLUS
CN 19-Norcholesta-1,3,5(10)-triene-23-yne-3,25-diol, 2-methoxy- (9CI) (CA INDEX NAME)

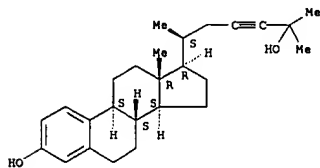
Absolute stereochemistry.



RN 305812-55-9 CAPLUS
CN 19-Norcholesta-1,3,5(10)-triene-23-yne-3,25-diol, (20S)- (9CI) (CA INDEX NAME)

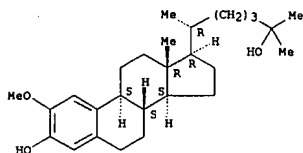
Absolute stereochemistry.

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



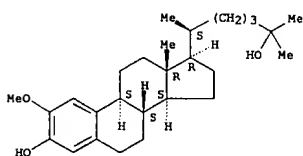
RN 305812-56-0 CAPLUS
CN 19-Norcholesta-1,3,5(10)-triene-3,25-diol, 2-methoxy-, (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-57-1 CAPLUS
CN 19-Norcholesta-1,3,5(10)-triene-3,25-diol, 2-methoxy-, (20S)- (9CI) (CA INDEX NAME)

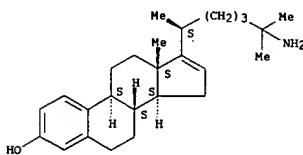
Absolute stereochemistry.



RN 305812-58-2 CAPLUS
CN 19-Norpregna-1,3,5(10)-triene-3-ol, 20-(5-hydroxy-5-methyl-1,3-hexadienyl)-, (20R)- (9CI) (CA INDEX NAME)

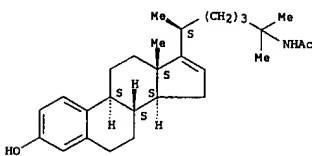
L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
CN 19-Norcholesta-1,3,5(10),16-tetraen-3-ol, 25-amino-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



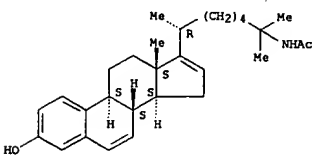
RN 305812-62-8 CAPLUS
CN Acetamide, N-[(20S)-3-hydroxy-19-norcholesta-1,3,5(10),16-tetraen-25-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



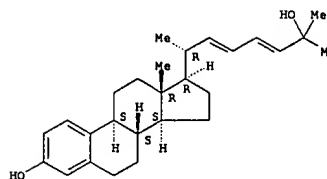
RN 305812-63-9 CAPLUS
CN Acetamide, N-[(6R)-6-(3-hydroxyestra-1,3,5(10),6,16-pentaen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



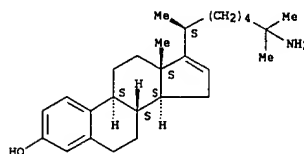
RN 305812-64-0 CAPLUS
CN 19-Norpregna-1,3,5(10),6,16-pentaen-3-ol, 20-(5-amino-5-methylhexyl)-, (20R)- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
Absolute stereochemistry.
Double bond geometry unknown.



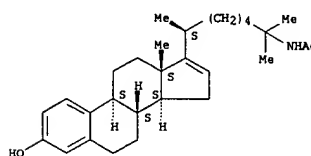
RN 305812-59-3 CAPLUS
CN 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-(5-amino-5-methylhexyl)-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



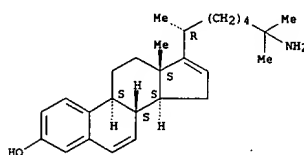
RN 305812-60-6 CAPLUS
CN Acetamide, N-[(6S)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-61-7 CAPLUS

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
Absolute stereochemistry.

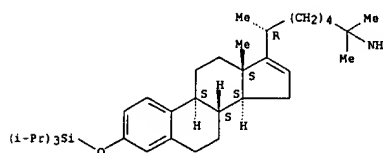


IT 305813-30-3P 305813-32-5P 305813-36-9P
305813-38-1P 305813-41-6P 305813-43-8P
305813-44-9P 305813-46-1P 305813-47-2P
305813-49-4P 305813-50-7P 305813-51-8P
305813-53-0P 305813-55-2P 305813-56-3P
305813-58-5P 305813-59-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of cholestane compds. with a c17-alkyl side chain and an arom. A-ring for use in cell modulating therapy)

RN 305813-30-3 CAPLUS
CN 19-Norpregna-1,3,5(10),16-tetraene-20-pentanamine, .alpha.,.alpha.-dimethyl-3-[[tris(1-methylethyl)silyl]oxy]-, (20R)- (9CI) (CA INDEX NAME)

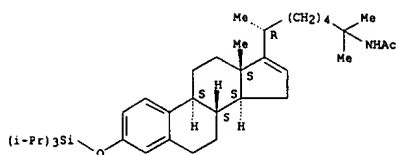
Absolute stereochemistry.



RN 305813-32-5 CAPLUS
CN Acetamide, N-[(6R)-1,1-dimethyl-6-[3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10),16-tetraen-17-yl]heptyl]- (9CI) (CA INDEX NAME)

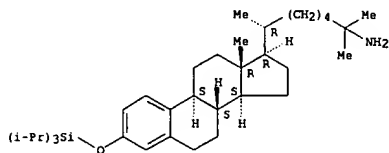
Absolute stereochemistry.

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



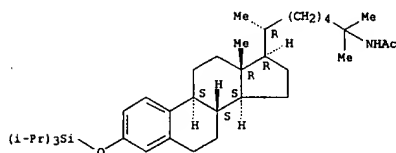
RN 305813-36-9 CAPLUS
 CN 19-Norpregna-1,3,5(10)-triene-20-pentanamine, .alpha.,.alpha.-dimethyl-3-[[tris(1-methylethyl)silyl]oxy]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



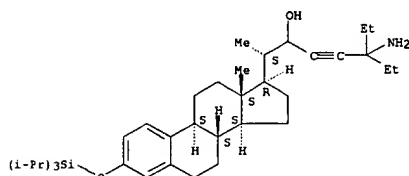
RN 305813-38-1 CAPLUS
 CN Acetamide, N-[(6R)-1,1-dimethyl-6-[(17.beta.)-3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10)-trien-17-yl]heptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



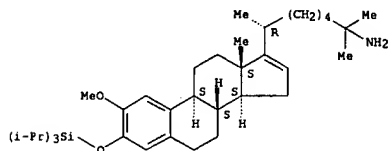
RN 305813-41-6 CAPLUS
 CN 19,26,27-Trinorcholesta-1,3,5(10)-trien-24-ol, 24-(2-propynyl)-3-[[tris(1-methylethyl)silyl]oxy]- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



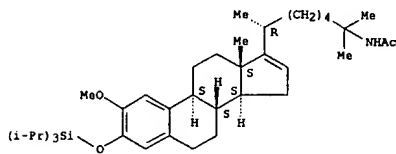
RN 305813-46-1 CAPLUS
 CN 19-Norpregna-1,3,5(10),16-tetraene-20-pentanamine, 2-methoxy-.alpha.,.alpha.-dimethyl-3-[[tris(1-methylethyl)silyl]oxy]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305813-47-2 CAPLUS
 CN Acetamide, N-[(6R)-6-[2-methoxy-3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10),16-tetraen-17-yl]-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

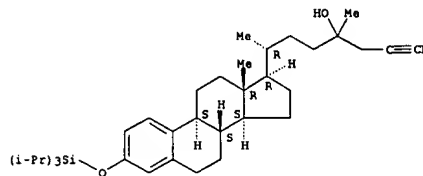


RN 305813-49-4 CAPLUS
 CN 19-Norpregna-1,3,5,7,9,16-hexaene-20-pentanamine, .alpha.,.alpha.-dimethyl-3-[[tris(1-methylethyl)silyl]oxy]-, (20R)- (9CI) (CA INDEX NAME)

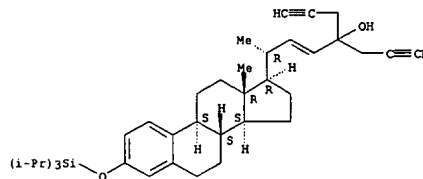
Absolute stereochemistry.

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

Absolute stereochemistry.



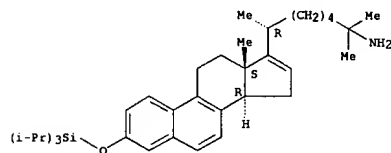
RN 305813-43-8 CAPLUS
 CN 5-Octen-1-yn-4-ol, 4-(2-propynyl)-7-[(17.beta.)-3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10)-trien-17-yl]-, (7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

RN 305813-44-9 CAPLUS
 CN 19-Norpregna-1,3,5(10)-triene-20-methanol, .alpha.,.alpha.-dimethyl-3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10)-trien-17-yl]-, (7R)- (9CI) (CA INDEX NAME)

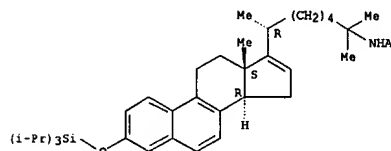
Absolute stereochemistry.

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



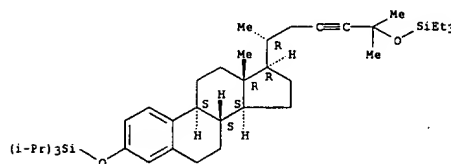
RN 305813-50-7 CAPLUS
 CN Acetamide, N-[(6R)-1,1-dimethyl-6-[3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5,7,9,16-hexaen-17-yl]heptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305813-51-8 CAPLUS
 CN Silane, [[25-[(triethylsilyl)oxy]-19-norcholesta-1,3,5(10)-trien-23-yn-3-yl]oxy]tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305813-53-0 CAPLUS
 CN 3,5-Octadien-2-ol, 2-methyl-7-[(17.beta.)-3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10)-trien-17-yl]-, (7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:814500 CAPLUS

DOCUMENT NUMBER: 133:350395

TITLE: Synthesis of cholestane compounds with a C17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy

INVENTOR(S): Hesse, Robert Henry; Setty, Sundara Katugam Srinivasasetty; Ramgopal, Malathi; Kugabaluooriar, Sanga

PATENT ASSIGNEE(S): Marsden, John, Christopher, UK; Research Institute for Medicine and Chemistry Inc.

SOURCE: PCT Int. Appl., 75 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000068246	A1	20001116	WO 2000-GB1813	20000511
V: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DO, EE, EG, ES, FI, FL, GB, GD, GE, GH, GM, GR, GU, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, BG, BR, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG EP 1179005 A1 20020213 EP 2000-927569 20000511 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO NO 2001005520 A 20020109 NO 2001-5520 20011112 GB 1999-10934 A 19990511 WO 2000-GB1813 W 20000511				

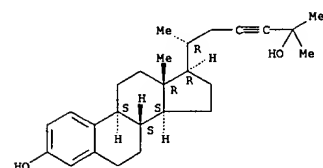
PRIORITY APPLN. INFO.: MARPAT 133:350395

OTHER SOURCE(S):

AB Synthesis of cholestane compds. (I) [R1 and R2, which may be the same or different, = alkyl, alkenyl, alkynyl; R3 = Me having alpha- or beta-configuration; R4 = H or an etherifying or esterifying group; R5 = H, OH, alkoxy; X = OR4, wherein R4 is as defined above, or NR6R7 wherein R6 = H, aliph. or araliph. org. group, acyl group comprising aliph., araliph. or aryl org. group linked to the nitrogen atom by way of a carbonyl group; R7 = H, alkyl; Y = (un)substituted alkylene, alkenylene, alkynylene; dotted lines signify that double bonds may be present at the 16(17)-position and/or either at the 6(7)- and 8(9)-positions or at the 7(8)-position] is disclosed for modulation of cell growth and differentiation, while having low calcemic activity. Thus, I [R1, R2 = Me; R3 = alpha-Me; R4, R5 = H; X = NHAc; Y = (CH2)4; DELTA-16 double bond] is prep'd. by reaction of 3-trisopropylsiloxy-19-norchole-1,3,5(10),16-tetraene-24-bromide with acetonitrile followed by redn. of nitrile to amine, methylation of amine with Me lithium, acetylation of the amine with acetic anhydride and desilylation with TBAF.

IT 305812-17-3P 305812-18-4P 305812-52-6P
 RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

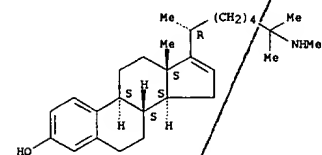


IT 305812-19-5P 305812-20-8P 305812-21-9P
 305812-22-0P 305812-23-1P 305812-24-2P
 305812-25-3P 305812-26-4P 305812-27-5P
 305812-28-6P 305812-29-7P 305812-30-8P
 305812-31-1P 305812-32-2P 305812-33-3P
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 305812-55-9P 305812-56-0P 305812-57-1P
 305812-58-2P 305812-59-3P 305812-60-6P
 305812-61-7P 305812-62-8P 305812-63-9P
 305812-64-0P

RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (synthesis of cholestane compds. with a C17-alkyl side chain and an arom. A-ring for use in cell modulating therapy)

RN 305812-19-5 CAPLUS
 CN 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-[5-methyl-5-(methylamino)hexyl]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



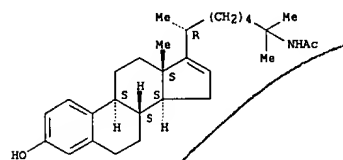
RN 305812-20-8 CAPLUS
 CN 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-[5-(dimethylamino)-5-methylhexyl]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (synthesis of cholestane compds. with a C17-alkyl side chain and an arom. A-ring for use in cell modulating therapy)

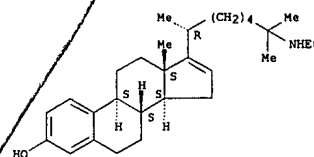
RN 305812-17-3 CAPLUS
 CN Acetamide, N-[(6R)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-18-4 CAPLUS
 CN 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-[5-(ethylamino)-5-methylhexyl]-, (20R)- (9CI) (CA INDEX NAME)

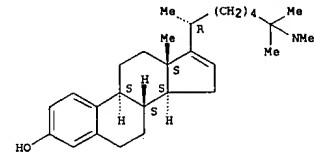
Absolute stereochemistry.



RN 305812-52-6 CAPLUS
 CN 19-Norcholesta-1,3,5(10)-trien-23-yne-3,25-diol (9CI) (CA INDEX NAME)

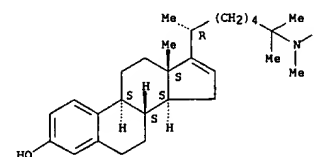
Absolute stereochemistry.

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)



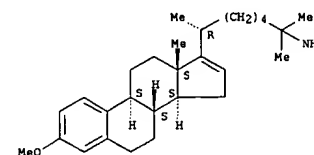
RN 305812-21-9 CAPLUS
 CN 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-[5-(ethylmethylamino)-5-methylhexyl]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-22-0 CAPLUS
 CN Acetamide, N-[(6R)-6-(3-methoxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

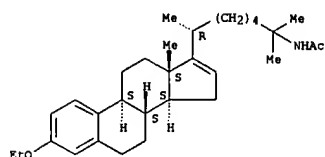
Absolute stereochemistry.



RN 305812-23-1 CAPLUS
 CN Acetamide, N-[(6R)-6-(3-ethoxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

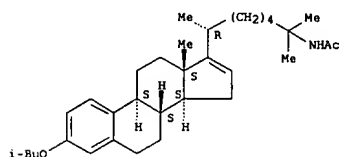
Absolute stereochemistry.

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)



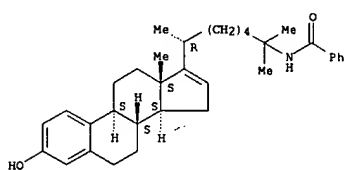
RN 305812-24-2 CAPLUS
 CN Acetamide, N-[(6R)-1,1-dimethyl-6-[3-(2-methylpropoxy)estra-1,3,5(10),16-tetraen-17-yl]heptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-25-3 CAPLUS
 CN Benzamide, N-[(6R)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

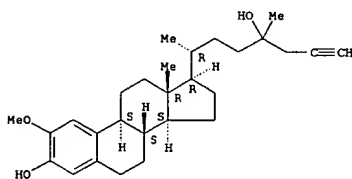


RN 305812-26-4 CAPLUS
 CN Benzeneacetamide, N-[(6R)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

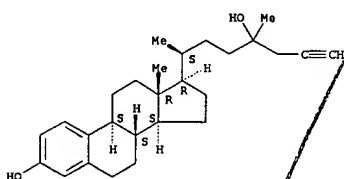
RN 305812-29-7 CAPLUS
 CN 19,26,27-Trinorcholesta-1,3,5(10)-triene-3,24-diol, 2-methoxy-24-(2-propynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-30-0 CAPLUS
 CN 19,26,27-Trinorcholesta-1,3,5(10)-triene-3,24-diol, 24-(2-propynyl)-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

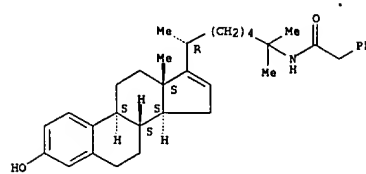


RN 305812-31-1 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-[3-hydroxy-3-(2-propynyl)-1-hexen-5-ynyl]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.

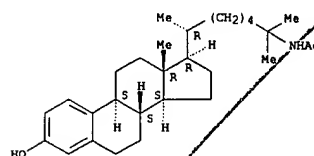
L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

Absolute stereochemistry.



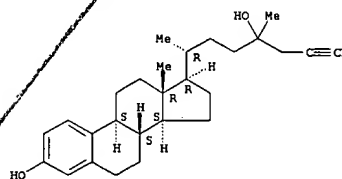
RN 305812-27-5 CAPLUS
 CN Acetamide, N-[(6R)-6-[(17.beta.)-3-hydroxyestra-1,3,5(10)-trien-17-yl]-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

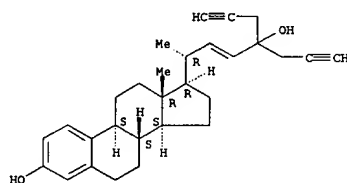


RN 305812-28-6 CAPLUS
 CN 19,26,27-Trinorcholesta-1,3,5(10)-triene-3,24-diol, 24-(2-propynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

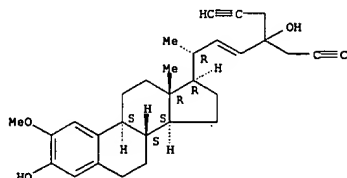


L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)



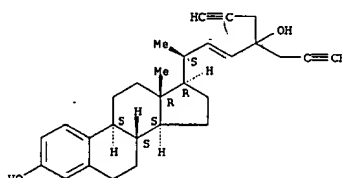
RN 305812-32-2 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-[3-hydroxy-3-(2-propynyl)-1-hexen-5-ynyl]-2-methoxy-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.



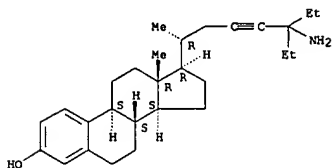
RN 305812-33-3 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-[3-hydroxy-3-(2-propynyl)-1-hexen-5-ynyl]-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.



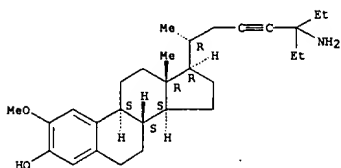
L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)
 RN 305812-34-4 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethyl-2-hexynyl)-, (20R)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-35-5 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethyl-2-hexynyl)-2-methoxy-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

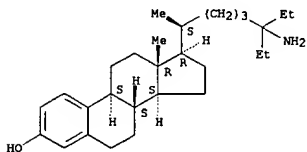


RN 305812-36-6 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethyl-2-hexynyl)-, (20S)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.

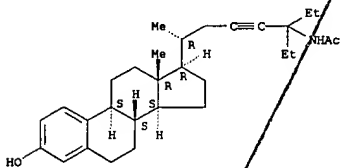
L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

Absolute stereochemistry.



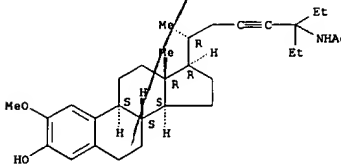
RN 305812-40-2 CAPLUS
 CN Acetamide, N-[(5R)-1,1-diethyl-5-[(17.beta.)-3-hydroxyestra-1,3,5(10)-trien-17-yl]-2-hexynyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



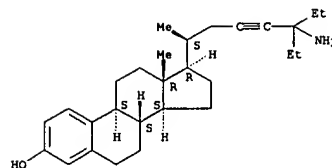
RN 305812-41-3 CAPLUS
 CN Acetamide, N-[(5R)-1,1-diethyl-5-[(17.beta.)-3-hydroxy-2-methoxyestra-1,3,5(10)-trien-17-yl]-2-hexynyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



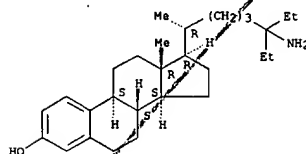
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 CN Acetamide, N-[(5S)-1,1-diethyl-5-[(17.beta.)-3-hydroxyestra-1,3,5(10)-trien-17-yl]-2-hexynyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)



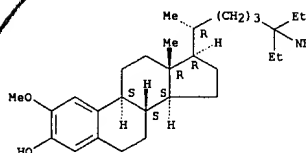
RN 305812-37-7 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethylhexyl)-, (20R)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-38-8 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethylhexyl)-2-methoxy-,
 (20R)- (9CI) (CA INDEX NAME)

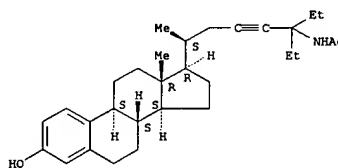
Absolute stereochemistry.



RN 305812-39-9 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethylhexyl)-, (20S)-
 (9CI) (CA INDEX NAME)

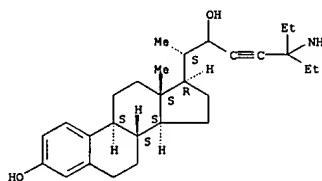
L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

Absolute stereochemistry.



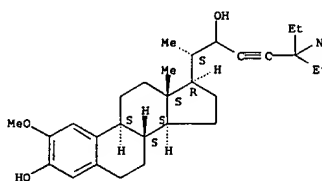
RN 305812-43-5 CAPLUS
 CN 19-Norpregna-1,3,5(10)-triene-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentynyl)-3-hydroxy-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-44-6 CAPLUS
 CN 19-Norpregna-1,3,5(10)-triene-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentynyl)-3-hydroxy-2-methoxy-, (20S)- (9CI) (CA INDEX NAME)

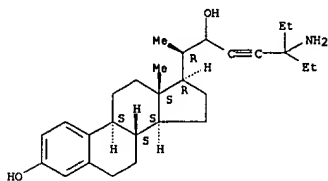
Absolute stereochemistry.



RN 305812-45-7 CAPLUS
 CN 19-Norpregna-1,3,5(10)-triene-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentynyl)-3-hydroxy-2-methoxy-, (20S)- (9CI) (CA INDEX NAME)

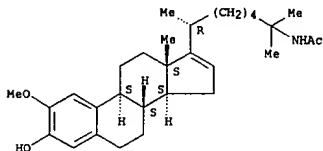
L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)
 pentynyl)-3-hydroxy-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



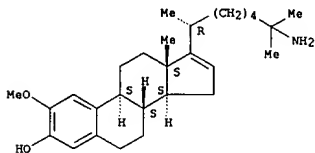
RN 305812-46-8 CAPLUS
 CN Acetamide, N-[(6R)-6-(3-hydroxy-2-methoxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

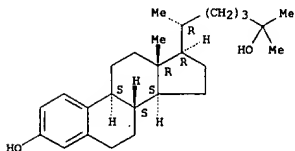


RN 305812-47-9 CAPLUS
 CN 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-(5-amino-5-methylhexyl)-2-methoxy-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

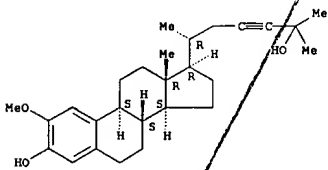


L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)



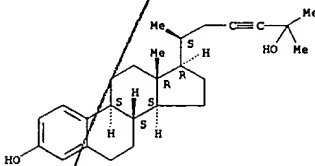
RN 305812-54-8 CAPLUS
 CN 19-Norcholesta-1,3,5(10)-trien-23-yne-3,25-diol, 2-methoxy-, (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-55-9 CAPLUS
 CN 19-Norcholesta-1,3,5(10)-trien-23-yne-3,25-diol, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



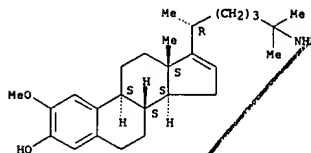
RN 305812-56-0 CAPLUS
 CN 19-Norcholesta-1,3,5(10)-triene-3,25-diol, 2-methoxy-, (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

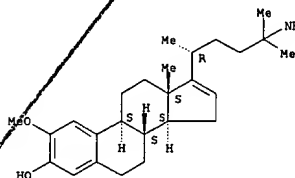
RN 305812-48-0 CAPLUS
 CN Acetamide, N-(3-hydroxy-2-methoxy-19-norcholesta-1,3,5(10),16-tetraen-25-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-49-1 CAPLUS
 CN 19,26,27-Trinorpregosta-1,3,5(10),16-tetraen-3-ol, 24-amino-2-methoxy-, (9CI) (CA INDEX NAME)

Absolute stereochemistry.

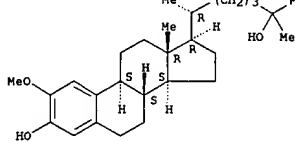


RN 305812-53-7 CAPLUS
 CN 19-Norcholesta-1,3,5(10)-triene-3,25-diol (9CI) (CA INDEX NAME)

Absolute stereochemistry.

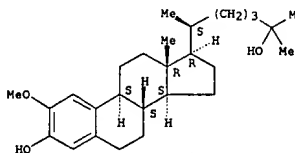


L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)



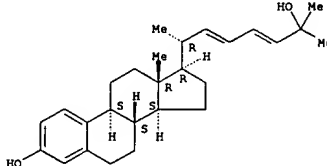
RN 305812-57-1 CAPLUS
 CN 19-Norcholesta-1,3,5(10)-triene-3,25-diol, 2-methoxy-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-58-2 CAPLUS
 CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(5-hydroxy-5-methyl-1,3-hexadienyl)-, (20R)- (9CI) (CA INDEX NAME)

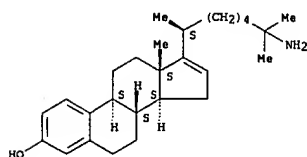
Absolute stereochemistry.
 Double bond geometry unknown.



RN 305812-59-3 CAPLUS
 CN 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-(5-amino-5-methylhexyl)-, (20S)- (9CI) (CA INDEX NAME)

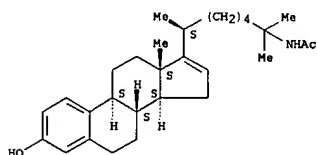
Absolute stereochemistry.

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)



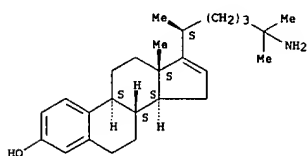
RN 305812-60-6 CAPLUS
 CN Acetamide, N-[(6S)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305812-61-7 CAPLUS
 CN 19-Norcholesta-1,3,5(10),16-tetraen-3-ol, 25-amino-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



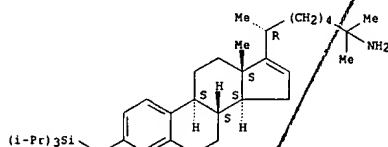
RN 305812-62-8 CAPLUS
 CN Acetamide, N-[(20S)-3-hydroxy-19-norcholesta-1,3,5(10),16-tetraen-25-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

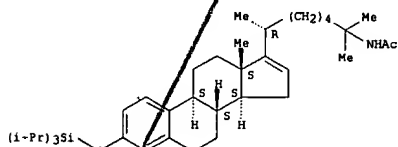
305813-51-6P 305813-53-0P 305813-55-2P
 305813-56-3P 305813-58-5P 305813-59-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (synthesis of cholestane compds. with a c17-alkyl side chain and an atom. A-ring for use in cell modulating therapy)
 RN 305813-30-3 CAPLUS
 CN 19-Norpregna-1,3,5(10),16-tetraene-20-pentanamine, .alpha.,.alpha.-dimethyl-3-[[tris(1-methylethyl)silyl]oxy]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305813-32-5 CAPLUS
 CN Acetamide, N-[(6R)-1,1-dimethyl-6-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10),16-tetraen-17-yl]heptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

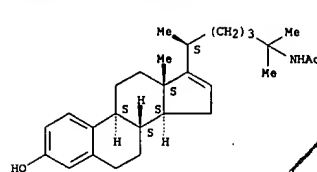


RN 305813-36-8 CAPLUS
 CN 19-Norpregna-1,3,5(10)-triene-20-pentanamine, .alpha.,.alpha.-dimethyl-3-[[tris(1-methylethyl)silyl]oxy]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

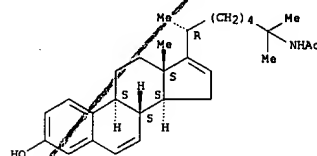


L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)



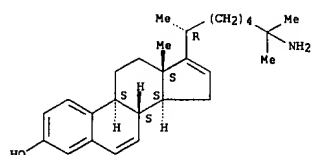
RN 305812-63-9 CAPLUS
 CN Acetamide, N-[(6R)-6-(3-hydroxyestra-1,3,5(10),6,16-pentaen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



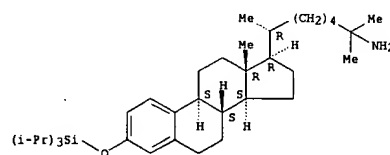
RN 305812-64-0 CAPLUS
 CN 19-Norpregna-1,3,5(10),6,16-pentaen-3-ol, 20-(5-amino-5-methylhexyl)-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



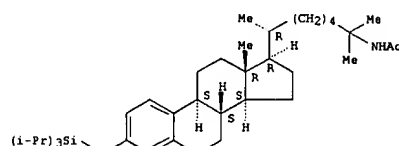
IT 305813-30-3P 305813-32-5P 305813-36-8P
 305813-38-1P 305813-41-6P 305813-43-8P
 305813-44-9P 305813-46-1P 305813-47-2P

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)



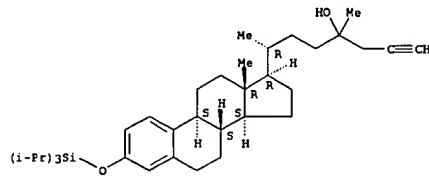
RN 305813-38-1 CAPLUS
 CN Acetamide, N-[(6R)-1,1-dimethyl-6-[(17.beta.)-3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10)-trien-17-yl]heptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305813-41-6 CAPLUS
 CN 19,26,27-Trinorcholesta-1,3,5(10)-trien-24-ol, 24-(2-propynyl)-3-[[tris(1-methylethyl)silyl]oxy]-, (9CI) (CA INDEX NAME)

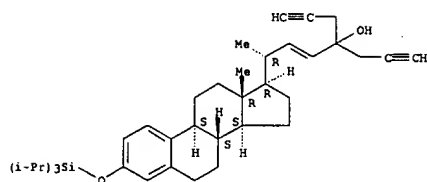
Absolute stereochemistry.



RN 305813-43-8 CAPLUS
 CN 5-Octen-1-yn-4-ol, 4-(2-propynyl)-7-[(17.beta.)-3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10)-trien-17-yl]-, (7R)- (9CI) (CA INDEX NAME)

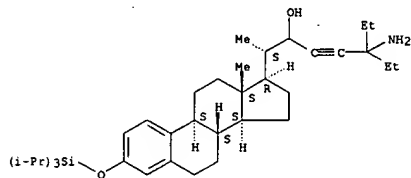
Absolute stereochemistry.

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)
Double bond geometry unknown.



RN 305813-44-9 CAPLUS
CN 19-Norpregna-1,3,5(10)-triene-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentynyl)-3-[[tris(1-methylethyl)silyl]oxy]-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

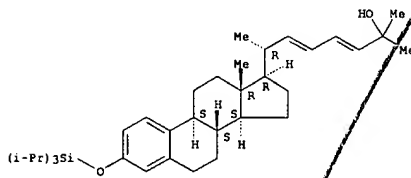


RN 305813-46-1 CAPLUS
CN 19-Norpregna-1,3,5(10),16-tetraene-20-pentanamine, 2-methoxy-.alpha.,.alpha.-dimethyl-3-[[tris(1-methylethyl)silyl]oxy]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

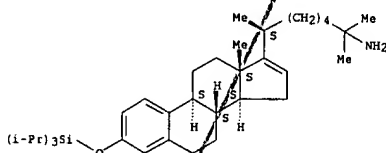
L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)
INDEX NAME

Absolute stereochemistry.
Double bond geometry unknown.



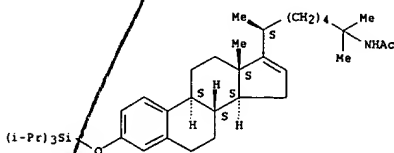
RN 305813-55-2 CAPLUS
CN 19-Norpregna-1,3,5(10),16-tetraene-20-pentanamine, .alpha.,.alpha.-dimethyl-3-[[tris(1-methylethyl)silyl]oxy]-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



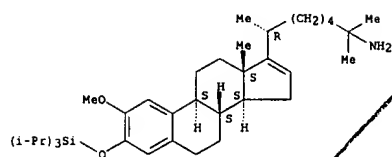
RN 305813-56-3 CAPLUS
CN Acetamide, N-[(6R)-1,1-dimethyl-6-[3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10),16-tetraen-17-yl]heptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



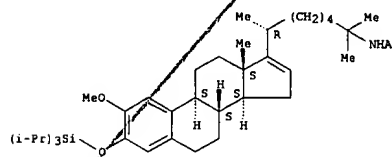
RN 305813-58-5 CAPLUS
CN 19-Norpregna-1,3,5(10),6,16-pentaene-20-pentanamine, .alpha.,.alpha.-dimethyl-3-[[tris(1-methylethyl)silyl]oxy]-, (20R)- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)



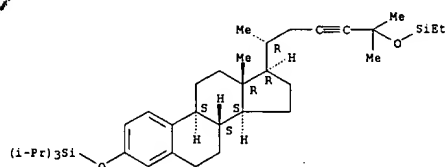
RN 305813-47-2 CAPLUS
CN Acetamide, N-[(6R)-6-[2-methoxy-3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10),16-tetraen-17-yl]-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 305813-51-8 CAPLUS
CN Silane, [[25-[[triethylsilyl]oxy]-19-norcholesta-1,3,5(10)-trien-23-yn-3-yl]oxy]tris(1-methylethyl)- (9CI) (CA INDEX NAME)

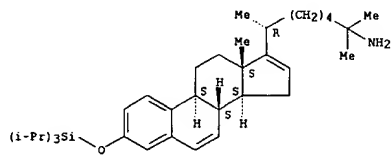
Absolute stereochemistry.



RN 305813-53-0 CAPLUS
CN 3,5-Octadien-2-ol, 2-methyl-7-[(17.beta.)-3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10)-trien-17-yl]-, (7R)- (9CI) (CA INDEX NAME)

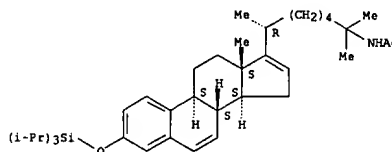
L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

Absolute stereochemistry.



RN 305813-59-6 CAPLUS
CN Acetamide, N-[(6R)-1,1-dimethyl-6-[3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10),6,16-pentaen-17-yl]heptyl]- (9CI) (CA INDEX NAME)

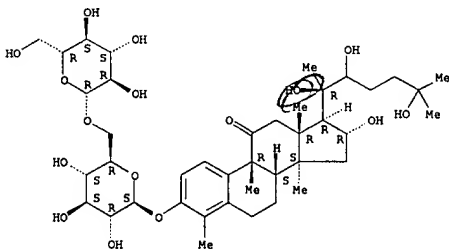
Absolute stereochemistry.



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

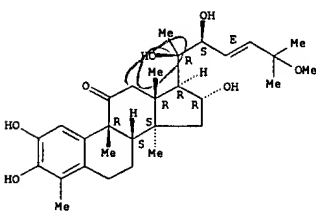
L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 1999:646426 CAPLUS
 DOCUMENT NUMBER: 132:2029
 TITLE: Studies on the constituents of *Cyclanthera pedata* fruits: isolation and structure elucidation of new triterpenoid saponins
 AUTHOR(S): De Tommasi, Nunziata; De Simone, Francesco; Speranza, Giovanna; Pizzi, Cosimo
 CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche Facoltà di Farmacia, Università di Salerno, Fisciano, 84084, Italy
 SOURCE: Journal of Agricultural and Food Chemistry (1999), 47(11), 4512-4519
 CODEN: JAFCAU; ISSN: 0021-8561
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The isolation of nine triterpenoid saponins, among them six new natural compounds, from the MeOH ext. of the fruits of *Cyclanthera pedata* is reported. All of the structures were elucidated by spectroscopic methods, including the concerted application of one-dimensional ¹H-¹H total correlation spectroscopy, ¹H-¹H nuclear Overhauser effect spectroscopy, and ¹³C-¹³C DEPT-NMR and two-dimensional NMR techniques (double-quantum filtered correlated spectroscopy, rotating-frame Overhauser enhancement spectroscopy, heteronuclear single quantum coherence, and heteronuclear multiple bond correlation). A comparative study of seeds and fruits has been also carried out.
 IT 251102-64-4
 RI: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence) (from *Cyclanthera pedata*)
 RN 251102-64-4 CAPLUS
 CN 19-Norcholesta-1,3,5(10)-trien-11-one, 3-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-16,20,22,25-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Currently available stereo shown.



L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 1994:73386 CAPLUS
 DOCUMENT NUMBER: 120:73386
 TITLE: New nor- and hepta nor-cucurbitacin glucosides from *Fevillea trilobata*
 AUTHOR(S): Valente, Ligia M. M.; Gunatilaka, A. A. Leslie; Glass, Thomas E.; Kingston, David G. I.; Pinto, Angelo C.
 CORPORATE SOURCE: Dep. Chem., Virginia Polytech. Inst. and State Univ., Blacksburg, VA, 24061-0212, USA
 SOURCE: Journal of Natural Products (1993), 56(10), 1772-8
 CODEN: JNPRDF; ISSN: 0163-3864
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB From the MeOH ext. of the seeds of *Fevillea trilobata* (Cucurbitaceae) were isolated fevicordin A glucoside (I), cayaononide B, cayaononide D, a new norcucurbitacin glucoside, and a new heptanorcucurbitacin glucoside. The structure of the new norcucurbitacin glucoside, andirobicin A glucoside (I), was established as 29-nor-1,2,3,4,5,10-dehydro-25-methoxy-2-O-.beta.-D-glucopyranosyl-3,16.alpha.,20R,22.xi.-tetrahydroxy-11-oxocucurbit-23-ene, and that of the novel heptanorcucurbitacin glucoside, andirobicin B glucoside, as 22,23,24,25,26,27,29-heptanor-1,2,3,4,5,10-dehydro-2-O-.beta.-D-glucopyranosyl-3,16.alpha.-dihydroxycucurbita-11,20-dione.
 IT 152340-77-7D, Andirobicin A, derivs.
 RI: BIOL (Biological study) (from *Fevillea trilobata*)
 RN 152340-77-7 CAPLUS
 CN 19-Norcholesta-1,3,5(10),23-tetraene-11-one, 2,3,16,20,22-pentahydroxy-25-methoxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,22S,23E)- (9CI) (CA INDEX NAME)

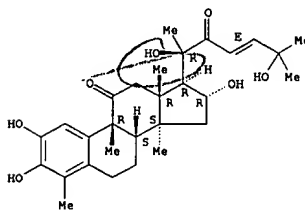
Absolute stereochemistry.
 Double bond geometry as shown.



L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)
 REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 1994:73357 CAPLUS
 DOCUMENT NUMBER: 120:73357
 TITLE: Constituents of tropical medicinal plants. 59. Constituents of *Fevillea cordifolia*: new norcucurbitacin and cucurbitacin glycosides
 AUTHOR(S): Achenbach, Hans; Waibel, Reiner; Hefter-Buehl, Ursula; Constenla, Manuel A.
 CORPORATE SOURCE: Inst. Pharm. Food Chem., Univ. Erlangen, Erlangen, D-91052, Germany
 SOURCE: Journal of Natural Products (1993), 56(9), 1506-19
 CODEN: JNPRDF; ISSN: 0163-3864
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The seeds of *F. cordifolia* yielded 11 new fevicordin-type 29-norcucurbitacins and two new cucurbitacin glycosides, which were isolated along with previous reported fevicordin A and its glucoside. Structure detns. are based on spectroscopic studies and on chem. interconversions.
 IT 152340-32-4D, Fevicordin C, derivs. 152340-33-5D, Fevicordin D, derivs. 152340-34-6D, Fevicordin E, derivs. 152340-35-7D, Fevicordin F, derivs.
 RI: BIOL (Biological study) (from *Fevillea cordifolia* seeds)
 RN 152340-32-4 CAPLUS
 CN 19-Norcholesta-1,3,5(10),23-tetraene-11,22-dione, 2,3,16,20,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

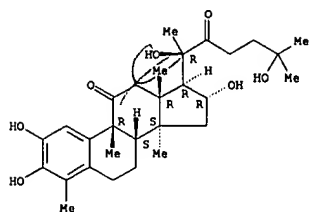
Absolute stereochemistry.
 Double bond geometry as shown.



RN 152340-33-5 CAPLUS
 CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 2,3,16,20,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

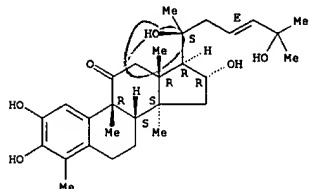
Absolute stereochemistry.

L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)



RN 152340-34-6 CAPLUS
 CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2,3,16,20,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.

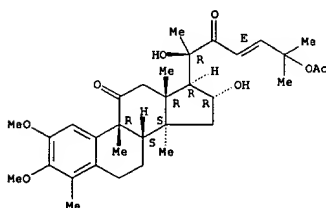


RN 152340-35-7 CAPLUS
 CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2,3,16,20,22,25-hexahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,22S,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.

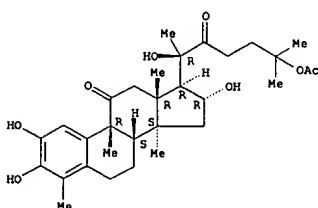
L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

Absolute stereochemistry.
 Double bond geometry as shown.

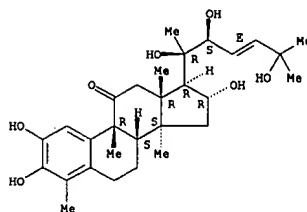


IT 152340-09-5, Fevicordin B
 RL: PROC (Process)
 (structure and isolation of, from *Fevillea cordifolia* seeds)
 RN 152340-09-5 CAPLUS
 CN 19-Norcholesta-1,3,5(10),23-tetraen-11,22-dione, 25-(acetyloxy)-2,3,16,20-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



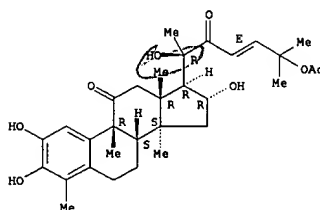
L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)



IT 111250-02-3, Fevicordin A
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BLOL (Biological study); USES (Uses)
 (from *Fevillea cordifolia*, antiinflammatory activity of)

RN 111250-02-3 CAPLUS
 CN 19-Norcholesta-1,3,5(10),23-tetraen-11,22-dione, 25-(acetyloxy)-2,3,16,20-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.

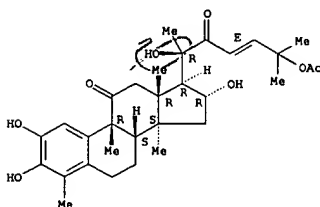


IT 151589-29-6P, 2,3-Di-O-methylfevicordin A
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 151589-29-6 CAPLUS
 CN 19-Norcholesta-1,3,5(10),23-tetraen-11,22-dione, 25-(acetyloxy)-16,20-dihydroxy-2,3-dimethoxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1987:617953 CAPLUS
 DOCUMENT NUMBER: 107:217953
 TITLE: Fevicordin A and fevicordin A glucoside, novel norcucurbitacins from *Fevillea cordifolia*
 Achenbach, Hans; Heftner-Buehl, Ursula; Constenla, Manuel A.
 AUTHOR(S):
 CORPORATE SOURCE: Inst. Pharm., Univ. Erlangen-Nuernberg, Erlangen, D-8520, Fed. Rep. Ger.
 SOURCE: Journal of the Chemical Society, Chemical Communications (1987), (6), 441-2
 CODEN: JCCCAT; ISSN: 0022-4936
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Fevicordin A glucoside and fevicordin A, isolated from the seeds of *Fevillea cordifolia*, have structures I (R = .beta.-glucosyl) and II (R = H), resp., on the basis of chem. and spectral data.
 IT 111250-02-3P, Fevicordin A
 RL: PREP (Preparation)
 (from *Fevillea cordifolia*, isolation and mol. structure detn. of)
 RN 111250-02-3 CAPLUS
 CN 19-Norcholesta-1,3,5(10),23-tetraen-11,22-dione, 25-(acetyloxy)-2,3,16,20-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1985:471583 CAPLUS

DOCUMENT NUMBER: 103:71583

TITLE:

A stereoselective synthesis of 1,2-diols from

alpha-hydroxyaldehydes

AUTHOR(S):

Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.;

Russell, Graeme B.; Horn, Dennis H. S.

CORPORATE SOURCE:

Dep. Chem., Univ. Wyoming, Laramie, WY, 82071, USA

SOURCE:

Tetrahedron Letters (1985), 26(9), 1189-92

CODEN: TETLAA; ISSN: 0040-4039

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 103:71583

AB

The addn. of LiC.tpbond.CMe20-THP (THP = tetrahydro-2H-pyran-2-yl) to (20R)-20-hydroxypregnane-20-carboxaldehyde I and II in the absence and in the presence of BF3 afforded predominantly 20R,22R-diols III and IV or 20R,22S-diols V and VI, resp., characteristic of ecdysones.

IT 97452-83-0P 97452-84-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

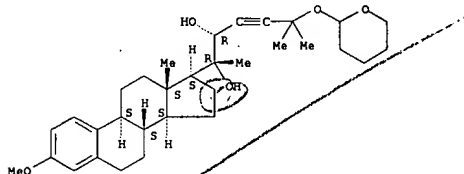
(prepn. and hydrolysis-hydrogenation of)

RN 97452-83-0 CAPLUS

CN 19-Norcholesta-1,3,5(10)-trien-23-yne-20,22-diol, 3-methoxy-25-

[(tetrahydro-2H-pyran-2-yl)oxy]-, (22R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 97452-84-1 CAPLUS

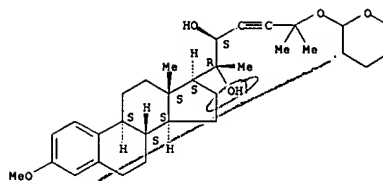
CN 19-Norcholesta-1,3,5(10)-trien-23-yne-20,22-diol, 3-methoxy-25-

[(tetrahydro-2H-pyran-2-yl)oxy]-, (22S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS

(Continued)



IT 97452-85-2P 97452-86-3P

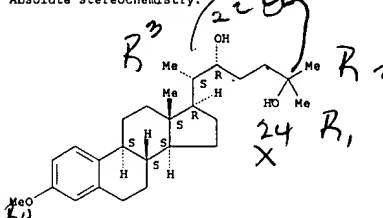
RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 97452-85-2 CAPLUS

CN 19-Norcholesta-1,3,5(10)-trien-22,25-diol, 3-methoxy-, (22R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 97452-86-3 CAPLUS

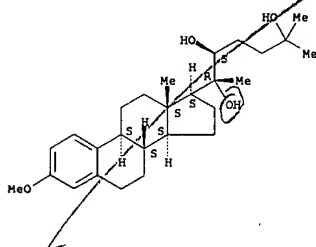
CN 19-Norcholesta-1,3,5(10)-trien-20,22,25-triol, 3-methoxy-, (22S)- (9CI)

(CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS

(Continued)



=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	29.72	178.29
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-3.91	-3.91

FILE 'REGISTRY' ENTERED AT 12:25:15 ON 03 APR 2003
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STRUCTURE FILE UPDATES: 2 APR 2003 HIGHEST RN 501410-52-2
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TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> d his

(FILE 'HOME' ENTERED AT 12:19:54 ON 03 APR 2003)

FILE 'REGISTRY' ENTERED AT 12:20:52 ON 03 APR 2003

L1 STRUCTURE UPLOADED
L2 6 S L1
L3 74 S L1 FULL

FILE 'CAPLUS' ENTERED AT 12:21:43 ON 03 APR 2003

L4 6 S L3

FILE 'REGISTRY' ENTERED AT 12:25:15 ON 03 APR 2003

=>

Uploading 491.str

L5 STRUCTURE UPLOADED

=> s l5 sub=13 full

FULL SUBSET SEARCH INITIATED 12:25:58 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 74 TO ITERATE

100.0% PROCESSED 74 ITERATIONS
SEARCH TIME: 00.00.01

74 ANSWERS

L6 74 SEA SUB=L3 SSS FUL L5

=> del l5- y

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	35.70	213.99
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-3.91

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FILE COVERS 1907 - 3 Apr 2003 VOL 138 ISS 14
FILE LAST UPDATED: 2 Apr 2003 (20030402/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L5 6 L3

=> s l5 not l4

L6 0 L5 NOT L4

=> file beil

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.42	214.41
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-3.91

FILE 'BEILSTEIN' ENTERED AT 12:26:28 ON 03 APR 2003
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FILE RELOADED ON OCTOBER 20, 2002

FILE LAST UPDATED ON MARCH 18, 2003

FILE COVERS 1771 TO 2002.

*** FILE CONTAINS 8,583,155 SUBSTANCES ***

>>> PLEASE NOTE: Reaction and substance documents are stored in different file segments. Use separate queries to search for reaction and substance data. When searching for bibliographic information you have the option to chose the file segment. (Use "/XXX.SUB" to search for a bibliographic term in substance documents. To restrict the search to reaction documents use "/XXX.RX".)
For additional information see HELP RXS. <<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
* FOR PRICE INFORMATION SEE HELP COST *

=> s l1 full

FULL SEARCH INITIATED 12:26:38 FILE 'BEILSTEIN'

FULL SCREEN SEARCH COMPLETED - 924 TO ITERATE

100.0% PROCESSED 924 ITERATIONS

7 ANSWERS

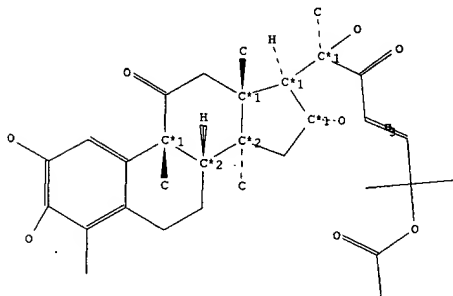
SEARCH TIME: 00.00.08

L7 7 SEA SSS FUL L1

=> d all 1-7

L7 ANSWER 1 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 7106735
 Chemical Name (CN): fevicordin A
 Autonom Name (AUN): acetic acid 5-hydroxy-1,1-dimethyl-4-oxo-5-(2,3,16-trihydroxy-4,9,13,14-tetramethyl-11-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-17-yl)-hex-2-enyl ester
 Molec. Formula (MF): C31 H42 O8
 Molecular Weight (MW): 542.67
 Lawson Number (LN): 10305, 1155
 File Segment (FS): Stereo compound
 Compound Type (CTYPE): isocyclic
 Constitution ID (CONSID): 6159741
 Tautomer ID (TAUTID): 6807808
 Beilstein Citation (BSO): 6-08
 Entry Date (DED): 1995/05/11
 Update Date (DUPD): 1995/05/11



Atom/Bond Notes:
 1. CIP Descriptor: R
 2. CIP Descriptor: S
 3. CIP Descriptor: E

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1

L7 ANSWER 1 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued)

J.Chem.Soc.Chem.Comm., CODEN: JCCCAT (6), <1987>, 441-442;
 BABS-5938125

L7 ANSWER 1 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued)

CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
INP	Isolation from Natural Product	1
RSTR	Related Structure	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXREA	Substance is Reaction Reactant	1

Related Structure:

RSTR: The author investigated the configuration
 Reference(s):
 1. Achenbach, Hans; Hefter-Buehl, Ursula; Constenla, Manuel A., J.Chem.Soc.Chem.Comm., CODEN: JCCCAT (6), <1987>, 441-442; BABS-5938125

Isolation from Natural Product:

INP: Fevillea cordifolia (Cucurbitaceae)
 Reference(s):
 1. Achenbach, Hans; Hefter-Buehl, Ursula; Constenla, Manuel A., J.Chem.Soc.Chem.Comm., CODEN: JCCCAT (6), <1987>, 441-442; BABS-5938125

Reaction:

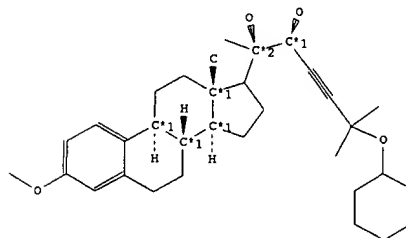
RX
 Reaction ID (.RID): 4023468
 Reactant BRN (.RBRN): 7106735
 Reactant (.RCT): fevicordin A
 Product BRN (.PBRN): 7103057
 Product (.PRO): 17-acetyl-2-hydroxy-3-methoxy-4,9,13,14-tetramethyl-6,7,8,9,12,13,14,15-octahydro-cyclopenta<a>phenanthren-11-one
 No. of React. Details (.NVAR): 1

Reaction Details:

RX
 Reaction RID (.RID): 4023468.1
 Reaction Classification (.CL): Preparation
 Reagent (.RG): NaBH4, NaIO4, H+/H2O
 Reference(s):
 1. Achenbach, Hans; Hefter-Buehl, Ursula; Constenla, Manuel A.,

L7 ANSWER 2 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 4728055
 CAS Reg. No. (RN): 97452-83-0, 97452-84-1
 Chemical Name (CN): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol
 Autonom Name (AUN): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol
 Molec. Formula (MF): C32 H46 O5
 Molecular Weight (MW): 510.71
 Lawson Number (LN): 17122, 6760, 289
 File Segment (FS): Stereo compound
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 4263612
 Tautomer ID (TAUTID): 4567456
 Beilstein Citation (BSO): 6-17
 Entry Date (DED): 1991/12/02
 Update Date (DUPD): 1991/12/02



Atom/Bond Notes:
 1. CIP Descriptor: S
 2. CIP Descriptor: R

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
RN	CAS Registry Number	2
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1

L7 ANSWER 2 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued)

FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	3
RXREA	Substance is Reaction Reactant	2
RXPRO	Substance is Reaction Product	1

Reaction:

RX

Reaction ID (.RID):	2442472
Reactant BRN (.RBRN):	4525023, 4133964
Reactant (.RCT):	2-hydroxy-2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol, 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol, 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol
Product BRN (.PBRN):	4728055, 4728054
Product (.PRO):	2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol

No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID):	2442472.1
Reaction Classification (.CL):	Preparation
Solvent (.SOL):	tetrahydrofuran
Temperature (.T):	-26 Cel
Note(s) (.COM):	Yield given. Yields of byproduct given
Reference(s):	1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.; Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

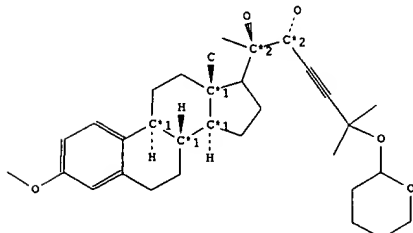
Reaction:

RX

Reaction ID (.ID):	2742338
Reactant BRN (.RBRN):	4728055
Reactant (.RCT):	2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-

L7 ANSWER 3 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN):	4728054
CAS Reg. No. (RN):	97452-83-0, 97452-84-1
Chemical Name (CN):	2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol
Autonom Name (AUN):	2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol
Molec. Formula (MF):	C32 H46 O5
Molecular Weight (MW):	510.71
Lawson Number (LN):	17122, 6760, 289
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	4263612
Tautomer ID (TAUTID):	4567455
Beilstein Citation (BSO):	6-17
Entry Date (DED):	1991/12/02
Update Date (DUPD):	1991/12/02



Atom/Bond Notes:

1. CIP Descriptor: S
2. CIP Descriptor: R

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
RN	CAS Registry Number	2
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1

L7 ANSWER 2 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued)

Product BRN (.PBRN):	4722039
Product (.PRO):	2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3,6-triol

No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID):	2742338.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	90 percent (BRN=4722039)
Reagent (.RGT):	70 percent HClO4
Solvent (.SOL):	H2O, methanol
Reference(s):	1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.; Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

Reaction:

RX

Reaction ID (.ID):	2742337
Reactant BRN (.RBRN):	4728055
Reactant (.RCT):	2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol, 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol
Product BRN (.PBRN):	4722038
Product (.PRO):	2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3,6-triol

No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID):	2742337.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	90 percent (BRN=4722038)
Reagent (.RGT):	70 percent HClO4
Solvent (.SOL):	H2O, methanol
Reference(s):	1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.; Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

L7 ANSWER 3 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued)

FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Reaction:

RX

Reaction ID (.ID):	2442472
Reactant BRN (.RBRN):	4525023, 4133964
Reactant (.RCT):	2-hydroxy-2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol, 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol, 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol
Product BRN (.PBRN):	4728055, 4728054
Product (.PRO):	2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol

No. of React. Details (.NVAR): 1

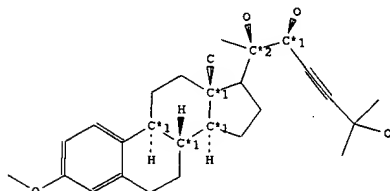
Reaction Details:

RX

Reaction RID (.RID):	2442472.1
Reaction Classification (.CL):	Preparation
Solvent (.SOL):	tetrahydrofuran
Temperature (.T):	-26 Cel
Note(s) (.COM):	Yield given. Yields of byproduct given
Reference(s):	1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.; Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

L7 ANSWER 4 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 4722039
 Chemical Name (CN): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-17-yl)-6-methylhept-4-yne-2,3,6-triol
 Autonom Name (AUN): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-17-yl)-6-methylhept-4-yne-2,3,6-triol
 Molec. Formula (MF): C27 H38 O4
 Molecular Weight (MW): 426.59
 Lawson Number (LN): 6760, 289
 File Segment (FS): Stereo compound
 Compound Type (CTYPE): isocyclic
 Constitution ID (CONSID): 4257630
 Tautomer ID (TAUTID): 4557405
 Beilstein Citation (BSO): 6-06
 Entry Date (DED): 1991/12/02
 Update Date (DUPD): 1991/12/02



Atom/Bond Notes:
 1. CIP Descriptor: S
 2. CIP Descriptor: R

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1

L7 ANSWER 4 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued)

Reaction Details:

RX

Reaction RID (.RID): 2737115.1
 Reaction Classification (.CL): Preparation
 Reagent (.RGT): H2
 Catalyst (.CAT): PtO2
 Reference(s):
 1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.; Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

L7 ANSWER 4 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued)

TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RKREA	Substance is Reaction Reactant	1
RKPRO	Substance is Reaction Product	1

Reaction:

RX

Reaction ID (.RID): 2742338
 Reactant BRN (.RBRN): 4728055
 Reactant (.RCT): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yl)oxy)-hept-4-yne-2,3-diol
 Product BRN (.PBRN): 4722039
 Product (.PRO): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-17-yl)-6-methylhept-4-yne-2,3,6-triol
 No. of React. Details (.NVAR): 1

Reaction Details:

RX

Reaction RID (.RID): 2742338.1
 Reaction Classification (.CL): Preparation
 Yield (.YDT): 90 percent (BRN=4722039)
 Reagent (.RGT): 70 percent HClO4
 Solvent (.SOL): H2O, methanol
 Reference(s):
 1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.; Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

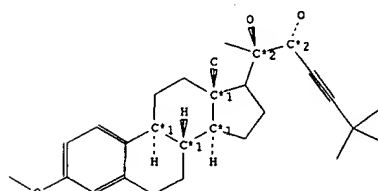
Reaction:

RX

Reaction ID (.RID): 2737115
 Reactant BRN (.RBRN): 4722039
 Reactant (.RCT): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-17-yl)-6-methylhept-4-yne-2,3,6-triol
 Product BRN (.PBRN): 4719751
 Product (.PRO): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-17-yl)-6-methylheptane-2,3,6-triol
 No. of React. Details (.NVAR): 1

L7 ANSWER 5 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 4722038
 Chemical Name (CN): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-17-yl)-6-methylhept-4-yne-2,3,6-triol
 Autonom Name (AUN): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-17-yl)-6-methylhept-4-yne-2,3,6-triol
 Molec. Formula (MF): C27 H38 O4
 Molecular Weight (MW): 426.59
 Lawson Number (LN): 6760, 289
 File Segment (FS): Stereo compound
 Compound Type (CTYPE): isocyclic
 Constitution ID (CONSID): 4257630
 Tautomer ID (TAUTID): 4557404
 Beilstein Citation (BSO): 6-06
 Entry Date (DED): 1991/12/02
 Update Date (DUPD): 1991/12/02



Atom/Bond Notes:
 1. CIP Descriptor: S
 2. CIP Descriptor: R

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1

L7 ANSWER 5 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued)

ED Entry Date 1
UPD Update Date 1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

Reaction:

RX
Reaction ID (.ID): 2742337
Reactant BRN (.RBRN): 4728055
Reactant (.RCT): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol
Product BRN (.PBRN): 4722038
Product (.PRO): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-hept-4-yne-2,3,6-triol
No. of React. Details (.NVAR): 1

Reaction Details:

RX
Reaction RID (.RID): 2742337.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 90 percent (BRN=4722038)
Reagent (.RGT): 70 percent HClO₄
Solvent (.SOL): H₂O, methanol
Reference(s):
1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.; Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

Reaction:

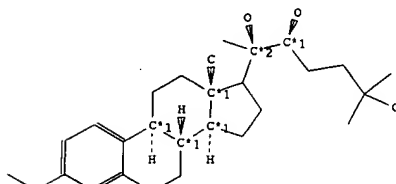
RX
Reaction ID (.ID): 2737114
Reactant BRN (.RBRN): 4722038
Reactant (.RCT): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-hept-4-yne-2,3,6-triol
Product BRN (.PBRN): 4719750
Product (.PRO): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-heptane-2,3,6-triol
No. of React. Details (.NVAR): 1

Reaction Details:

RX

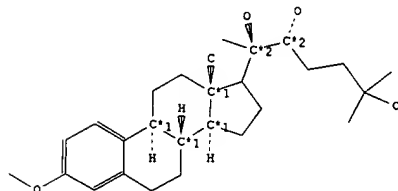
L7 ANSWER 6 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 4719751
Beilstein Pref. RN (BPR): 97452-86-3
CAS Reg. No. (RN): 97452-86-3
Chemical Name (CN): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-heptane-2,3,6-triol
Autonom Name (AUN): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methyl-heptane-2,3,6-triol
Molec. Formula (MF): C₂₇ H₄₂ O₄
Molecular Weight (MW): 430.63
Lawson Number (LN): 6704, 289
File Segment (FS): Stereo compound
Compound Type (CTYPE): isocyclic
Constitution ID (CONSID): 4257631
Tautomer ID (TAUTID): 4555354
Beilstein Citation (BSO): 6-06
Entry Date (DED): 1991/12/02
Update Date (DUPD): 1993/03/20



L7 ANSWER 7 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 4719750
 Beilstein Pref. RN (BPR): 97452-86-3
 CAS Reg. No. (RN): 97452-86-3
 Chemical Name (CN): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methylheptane-2,3,6-triol
 Autonom Name (AUN): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methylheptane-2,3,6-triol
 C27 H42 O4
 Molec. Formula (MF):
 Molecular Weight (MW): 430.63
 Lawson Number (LN): 6704, 289
 File Segment (FS): Stereo compound
 Compound Type (CTYPE): isocyclic
 Constitution ID (CONSID): 4257631
 Tautomer ID (TAUTID): 4555353
 Beilstein Citation (BSO): 6-06
 Entry Date (DED): 1991/12/02
 Update Date (DUPD): 1993/03/20



Atom/Bond Notes:
 1. CIP Descriptor: S
 2. CIP Descriptor: R

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
PW	Formular Weight	1

L7 ANSWER 7 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued)

Code	Name	Occurrence
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
NMR	Nuclear Magnetic Resonance	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Nuclear Magnetic Resonance:

NMR

Description (.KW):	Chemical shifts
Nucleus (.NUC):	13C
Solvents (.SOL):	pyridine-d5

Reference(s):

1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.; Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

Reaction:

RX

Reaction ID (.ID):	2737114
Reactant BRN (.RBRN):	4722038
Reactant (.RCT):	2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methylhept-4-yne-2,3,6-triol
Product BRN (.PBRN):	4719750
Product (.PRO):	2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)-6-methylheptane-2,3,6-triol
No. of React. Details (.NVAR):	1

Reaction Details:

RX

Reaction RID (.RID):	2737114.1
Reaction Classification (.CL):	Preparation
Reagent (.RG):	H2
Catalyst (.CAT):	PtO2
Reference(s):	1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.; Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

=> d his

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FILE 'REGISTRY' ENTERED AT 12:20:52 ON 03 APR 2003

L1 STRUCTURE UPLOADED

L2 6 S L1

L3 74 S L1 FULL

FILE 'CAPLUS' ENTERED AT 12:21:43 ON 03 APR 2003

L4 6 S L3

FILE 'REGISTRY' ENTERED AT 12:25:15 ON 03 APR 2003

FILE 'CAPLUS' ENTERED AT 12:26:14 ON 03 APR 2003

L5 6 S L3

L6 0 S L5 NOT L4

FILE 'BEILSTEIN' ENTERED AT 12:26:28 ON 03 APR 2003

L7 7 S L1 FULL

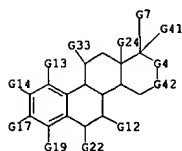
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L10 ANSWER 1 OF 16 MARPAT COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 139:73420 MARPAT
 TITLE: Preparation of anti-estrogenic steroids, and associated pharmaceutical compositions and methods of use
 INVENTOR(S): Tanabe, Masato; Peters, Richard H.; Chao, Wan-Ru; Jong, Ling
 PATENT ASSIGNEE(S): SRI International, USA
 SOURCE: U.S., 50 pp., Cont. of U.S. Ser. No. 220,408.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 4
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6503896	B1	20030107	US 2001-872826	20010531
US 6054446	A	20000425	US 1997-998877	19971224
US 6281205	B1	20010828	US 1998-220408	19981224
			US 1997-998877	19971224
			US 1998-220408	19981224

PRIORITY APPLN. INFO.:
 AB Steroid derivs., such as I and II [R = C, N; dashed lines = optional double bond; X, X1 = hydrocarbyl, generally including at least one O, S, N atom in the form of -O-, -S-, -NH- or -N(alkyl)-linkage; XX1 = heterocyclic ring; R1 = H, alkyl; R2 = H, OH, alkyl, alkoxy, thioalkyl; R3-R5, R7, R9 = H, alkyl; R6 = H, alkyl, acyl; R8 = H, OH, alkoxy; R10 = Me, Et; R20 = :CH(CH2)m-O-L-(CH2)p-NR21R22, :CH(CH2)m-O-p-(sub)C6H4-(CH2)p-NR21R22; m = 0-5; p = 0-6; L = cyclic or heterocyclic ring; R21, R22 = alkyl; R21R22 = cycloalkyl, heterocycloalkyl], or a pharmaceutically acceptable salt thereof, were prepd to treat a variety of disorders, particularly estrogen-dependent disorders including prostatic cancer. Thus, (E)-3-hydroxy-21-[2'-(piperazinyl)ethoxy]-19-norpregna-1,3,5(10),17(20)-tetraene (III) was prepd. via a multistep synthetic sequence starting from estrone, vinylmagnesium bromide, and 1-(2-hydroxyethyl)piperazine. III exhibited 100% antiestrogenic activity against Human Ishikawa cells at 10 μ M concn. Therapeutic methods and pharmaceutical compns. were also provided.

MSTR 3

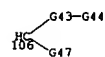


G4 = 28

L10 ANSWER 1 OF 16 MARPAT COPYRIGHT 2003 ACS (Continued)



G17 = OH
 G24 = Me
 G41 = 106



G43 = Ak (S0)
 G45 = O
 G47 = alkyl<(1-24)> (S0)
 DER: or pharmaceutically acceptable salts or esters
 MPL: disclosure
 NTE: oxo substitution also disclosed

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

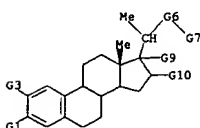
L10 ANSWER 2 OF 16 MARPAT COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 137:370278 MARPAT
 TITLE: Preparation of substituted prena-1,3,5(10)-triene derivatives for pharmaceutical use
 INVENTOR(S): Hesse, Robert Henry; Setty, Sundara Katugam
 PATENT ASSIGNEE(S): Srinivasasetty; Pechet, Maurice Murdoch; Gile, Michael
 SOURCE: Marsden, John Christopher, UK; Research Institute for Medicine and Chemistry Inc.
 DOCUMENT TYPE: FCT Int. Appl., 28 pp.
 CODEN: PIXXD2
 LANGUAGE: Patent
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002092100	A1	20021121	WO 2002-GB2210	20020513

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:
 AB Pregna-1,3,5(10)-triene derivs., such as I [R1 = H, hydroxy protecting group; R2 = OH, CHO, alkoxy, alkenyl, alkyl, etc.; R3 = .alpha.-, .beta.-Me; X = C1-3 alkylene group, bond; Y = C(R4)(R5)NR6R7; R4, R5 = H, alkyl, alkenyl and alkenyl groups, such that the total carbon content of R4 and R5 does not exceed three atoms; R6 = H, aliph. or araliph. org. group, acyl, etc.; C16-C17 = satd., unsatd.], were prepd. for a variety of therapeutic uses, such as modulating cell activity, including antiproliferative and antiangiogenic effects. Thus, prena-1,3,5(10)-triene derivs. II (Y = NH2, NHCOMe) were prepd. via a multistep synthetic series starting from 2-methoxy-3-[[tris(1-methylethyl)silyl]oxy]-estra-1,3,5(10)-trien-17-one and ethyltriphenylphosphonium bromide. Pharmaceutical compns. of the prepd. compds. were discussed, but specific pharmaceutical activity testing data was not presented.

MSTR 1



G1 = OH
 G3 = OH
 G6 = alkylene<(1-3)>
 G7 = 30

L10 ANSWER 2 OF 16 MARPAT COPYRIGHT 2003 ACS (Continued)



G8 = alkyl<(1-3)>
 G13 = NH2
 MPL: claim 1
 NTE: total carbon carbon content of G8 does not exceed three atoms
 NTE: substitution is restricted

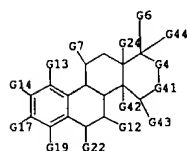
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 16 MARPAT COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 136:232440 MARPAT
 TITLE: Preparation of novel anti-estrogenic steroids
 INVENTOR(S): Tanabe, Masato; Peters, Richard H.; Chao, Wan-ru;
 Jang, Ling
 PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 56 pp., Cont.-in-part of U.S.
 6,281,205.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 4
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002032180	A1	20020314	US 2001-872825	20010531
US 6054446	A	20000425	US 1997-998877	19971224
US 6281205	B1	20010828	US 1998-220408	19981224
PRIORITY APPLN. INFO.:			US 1997-998877	19971224

PRIORITY APPLN. INFO.:

AB Novel antiestrogenic compds., e.g. of formula I: X = hydrocarbon contg. O, S or N, etc.; X1 = H, hydrocarbon contg. O, S or N, etc.; XX1 = heterocycles; Y = C, N; R1 = H, alkyl, halo, etc.; R2 = H, OH, alkyl, alkenyl, aryl, etc.; R3 = H, OH, CN, alkyl, etc.; R4 = H, OH, alkyl; R5 = H, alkoxy, halo, CN, etc.; R6 = H, alkyl, acyl, SO2NH2; R7 = H, halo, nitro, CHO, allyl, etc.; R8 = H, OH, etc.; R9 = H, alkyl; R10 = Me, Et, etc., are prep'd. which are useful to treat a variety of disorders, particularly estrogen-dependent disorders. Preferred compds. have a 1,3,5-estratriene nucleus, and are substituted at the C-17 or C-11 position with a mol. moiety which renders the compds. effective to competitively block the binding of estradiol to its receptor. The preferred compds. are pharmaceutical compns. are provided as well. Thus, II citrate salt was prep'd. from 7.alpha.-methyl-17.beta.-hydroxyethyl-1,3,5-estratrien-3-ol, vanillin and diethylamine. II citrate salt showed significant growth suppressive activity against MCF-7 tumor in mice at 10 mg/kg/day.

MSTR 3

G3 - 23

L10 ANSWER 5 OF 16 MARPAT COPYRIGHT 2003 ACS (Continued)



G4 - 28



G17 - OH
G24 - Me
G25 - Ak (SR (1-) G26)
G27 - O
G31 - alkyl<(1-24)>
MPE: claim 20
NTE: or pharmaceutically acceptable salts or esters

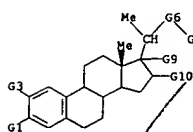
L10 ANSWER 6 OF 16 MARPAT COPYRIGHT 2003 ACS

TITLE: PREPARATION OF 2-SUBSTITUTED PREGNA-1,3,5(10)-TRIENE
 AND CHOLA-1,3,5(10)-TRIENE DERIVATIVES WITH
 ANTIPROLIFERATIVE AND ANTIANGIOGENIC ACTIVITY
 INVENTOR(S): HESSE, ROBERT HENRY; SETTY, SUNDARA KATUGAM
 Srinivasasethy; PECHET, MAURICE MURDOCH; GILE, MICHAEL
 PATENT ASSIGNEE(S): MARDEN, JOHN CHRISTOPHER, UK; RESEARCH INSTITUTE FOR
 MEDICINE AND CHEMISTRY INC.
 SOURCE: PCT INT. APPL., 40 PP.
 CODEN: P1XXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001085755	A1	20011115	WO 2001-GB2103	20010551
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, EE, ES, FI, FR, GB, GE, GM, GR, HU, IL, IN, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LV, LU, MA, MD, MG, MK, MN, MW, MX, NZ, NO, NZ, OM, PA, PE, PG, PH, PI, PT, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, BY, KG, KZ, MD, MU, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, NZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BU, CF, CG, CI, CM, CA, GN, GW, ML, MR, NE, SN, TD, TG			
EP 1287017	A1	20030305	EP 2001-928120	20010551
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, PT, SE, MC, PT, IE, SI, LT, LV, LU, FI, NO, HK, CY, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, EE, ES, FI, FR, GB, GE, GM, GR, HU, IL, IN, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LV, LU, MA, MD, MG, MK, MN, MW, MX, NZ, NO, NZ, OM, PA, PE, PG, PH, PI, PT, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, BY, KG, KZ, MD, MU, RU, TJ, TM			
NO 2002005392	A	20030109	US 2000-5392	20020111
PRIORITY APPLICATION. INFO:			US 2002-3462P	20020051

AB Compds. of formula I [R1 = H, protecting group; R2 = OH, alkoxy, CHO, alkenyl, etc.; X = alkylene, bond; Y = CHO, (substituted) CH2OH, etc.] are prepd. which exhibit potent cell modulating activity, including antiproliferative and antiangiogenic effects. Thus, 2-methoxy-3-triisopropylsilyloxy-19-norpregn-1,3,5(10),17(20)-2-tetraene (prepn. given) is reacted with Me acrylate, reduced with LiAlH₄, and desilylated with TBAF to give II.

NETR 1



G1 = OH
G3 = OH
G6 = alkylene<(1-3)>
G7 = 30

L10 ANSWER 6 OF 16 MARPAT COPYRIGHT 2003 ACS (Continued)



G8 = alkyl<(1-3)>
MPL: claim 1
NTE: total carbon carbon content of G8 does not exceed three atoms
NTE: substitution is restricted

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

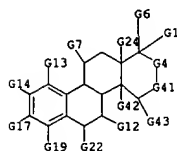
L10 ANSWER 7 OF 16 MARPAT COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 135:195698 MARPAT
 TITLE: Preparation of anti-estrogenic steroids, and associated pharmaceutical compositions and methods of use
 INVENTOR(S): Tanabe, Masato; Peters, Richard H.; Chao, Wan-ru; Jong, Ling
 PATENT ASSIGNEE(S): Sri International, USA
 SOURCE: U.S., 50 pp., Cont.-in-part of U.S. 6,054,446. CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 4
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6281205	B1	20010828	US 1998-220408	19981224
US 6054446	A	20000425	US 1997-998877	19971224
US 2002032180	A1	20020314	US 2001-872825	20010531
US 6503896	B1	20030107	US 2001-872826	20010531
US 2002032181	A1	20020314	US 2001-918890	20010730
US 6455517	B1	20020924		

PRIORITY APPLN. INFO.: US 1997-998877 19971224
 US 1998-220408 19981224

AB Novel antiestrogenic compds. are prepd. which are useful to treat a variety of disorders, particularly estrogen-dependent disorders. Preferred compds. have a 1,3,5(10)-estratriene nucleus, and are substituted at the C-17 or C-11 position with a mol. moiety which renders the compds. effective to competitively block the binding of estrogen to its receptor. Particularly preferred compds. are 17-desoxy-1,3,5(10)-estratrienes, e.g. of formula I [R1 = H, alkoxy, halo, CN, etc.; R2 = H, OH, alkyl, etc.; R3 = H, alkyl, acyl, SO2NH2, etc.; R4, R5 = H, alkyl, heterocyclyl; etc.; L = (substituted) five- or six-membered cyclic moiety; m = 1-6; p = 0-6]. Thus, II citrate salt was prepd. and showed strong growth inhibitory activity against MCF-7 human mammary tumor at 10 mg/kg/day. Therapeutic methods and pharmaceutical compns. are provided as well.

MYSTR 1



G3 = 23

L10 ANSWER 7 OF 16 MARPAT COPYRIGHT 2003 ACS (Continued)



G4 = 28



G17 = OH
 G24 = Me
 G25 = Ak (SR (1-) G26)
 G27 = O
 G31 = alkyl<(1-24)>
 MPL: claim 3
 NTE: or pharmaceutically acceptable salts or esters
 NTE: oxo substitution also claimed
 NTE: also incorporates broader disclosure

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

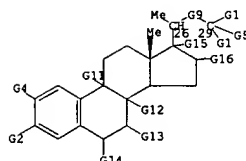
L10 ANSWER 8 OF 16 MARPAT COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 133:350395 MARPAT
 TITLE: Synthesis of cholestane compounds with a C17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy
 INVENTOR(S): Hesse, Robert Henry; Setty, Sundara Katugam Srinivasasetty; Ramgopal, Malathi; Kugabaluooriar, Sanga
 PATENT ASSIGNEE(S): Marsden, John, Christopher, UK; Research Institute for Medicine and Chemistry Inc.
 SOURCE: PCT Int. Appl., 75 pp. CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000068246	A1	20001116	WO 2000-GB1813	20000511
V: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DE, DE, DK, DM, DZ, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1179005	A1	20020213	EP 2000-927569	20000511
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
NO 2001005520	A	20020109	NO 2001-5520	20011112
GB 1999-10934 19990511				
WO 2000-GB1813 20000511				

AB Synthesis of cholestane compds. (I) [R1 and R2, which may be the same or different, = alkyl, alkenyl, alkynyl; R3 = Me having .alpha.- or .beta.-configuration; R4 = H or an etherifying or esterifying group; R5 = H, OH, alkoxy; X = OR4, wherein R4 is as defined above, or NR6R7 wherein R6 = H, aliph. or araliph. org. group, acyl group comprising aliph., araliph. or aryl org. group linked to the nitrogen atom by way of a carbonyl group; R7 = H, alkyl; Y = (un)substituted alkylene, alkenylene, alkynylene; dotted lines signify that double bonds may be present at the 16(17)-position and/or either at the 6(7)- and 8(9)-positions or at the 7(8)-position] is disclosed for modulation of cell growth and differentiation, while having low calcemic activity. Thus, I [R1,R2 = Me; R3 = .alpha.-Me; R4,R5 = H; X = NHAc; Y = (CH2)4; .DELTA.16 double bond] is prepd. by reaction of 3-triisopropylsilyloxy-19-norchole-1,3,5(10),16-tetraene-24-bromide with acetonitrile followed by redn. of nitrile to amine, methylation of amine with Me lithium, acetylation of the amino with acetic anhydride and desilylation with TBAF.

MYSTR 1

L10 ANSWER 8 OF 16 MARPAT COPYRIGHT 2003 ACS (Continued)



G1 = loweralkyl
 G2 = OH
 G9 = loweralkylene (SO G10)
 G10 = OH
 MPL: claim 1

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 9 OF 16 MARPAT COPYRIGHT 2003 ACS

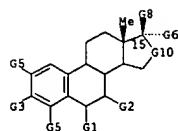
ACCESSION NUMBER: 132:152024 MARPAT
 TITLE: Preparation of steroids as inhibitors of type 3
 3.alpha.-hydroxysteroid dehydrogenase
 INVENTOR(S): Labrie, Fernand; Mercand, Yves; Gauthier, Sylvain;
 Provencher, Louis; Luu-The, Van
 PATENT ASSIGNEE(S): Endorecherche, Inc., Can.
 SOURCE: PCT Int. Appl., 140 pp.
 CODEN: PIXX02
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000007576	A2	20000217	WO 1999-CA724	19990806
WO 2000007576	A3	20000330		
V: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2339368	AA	20000217	CA 1999-2339368	19990806
AU 9951449	A1	20000228	AU 1999-51449	19990806
EP 1102582	A2	20010530	EP 1999-936218	19990806
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002522380	T2	20020723	JP 2000-563261	19990806
NO 2001000651	A	20010405	NO 2001-651	20010207
PRIORITY APPLN. INFO.: US 1998-95623P 19980807				
WO 1999-CA724 19990806				

AB Novel methods of treating and/or inhibiting development of prostatic cancer, benign prostatic hyperplasia, prostatitis, acne, seborrhea, hirsutism or androgenic alopecia utilize inhibitors of type 3 3.alpha.-hydroxysteroid dehydrogenase alone or in combination with other active pharmaceuticals such as inhibitors of type 5 17.beta.-hydroxysteroid dehydrogenase. The inhibitors, of formula I [R1 = OH, acyloxy, alkoxy, amido, etc.; R2, R4 = H, CN, F, Cl, Br, NO2; R3 = alkoxy, acyloxy, alkoxyacetyloxy, OH, carbamate; R5 = H, alkyl, etc.; R1R5 = O, lactone ring; R6, R7 = H, alkyl, benzyl; R6R7 = cycloalkene], are prepd. Thus, I showed 98% inhibition of the transformation of 4-dione by type 3 3.alpha.-HSD. Pharmaceutical compns. contg. I are described.

MSTR 1

L10 ANSWER 9 OF 16 MARPAT COPYRIGHT 2003 ACS (Continued)



G3 = alkoxy<(1-20)>
 G6 = hydrocarbyl<(2-14)> (SO (1-1) G7)
 G7 = CO2H / alkoxy<(1-3)> / alkyl<(1-5)>
 G10 = 35



MPL: claim 3

L10 ANSWER 10 OF 16 MARPAT COPYRIGHT 2003 ACS

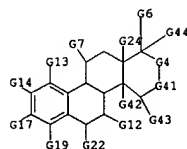
ACCESSION NUMBER: 131:88084 MARPAT
 TITLE: Preparation of novel antiestrogenic steroids
 INVENTOR(S): Tanabe, Masato; Peters, Richard H.; Chao, Wan-Ru;
 Jong, Ling
 PATENT ASSIGNEE(S): SRI International, USA
 SOURCE: PCT Int. Appl., 142 pp.
 CODEN: PIXX02
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 4
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9933859	A2	19990708	WO 1998-US27406	19981223
WO 9933859	A3	19991223		
V: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6054446	A	20000425	US 1997-998877	19971224
AU 9920104	A1	19990719	AU 1999-20104	19981223
AU 749597	B2	20020627		
EP 1056768	A2	20001206	EP 1998-964882	19981223
EP 1056768	B1	20030319		
R: DE, FR, GB, IT, NL				
JP 2001525855	T2	20011211	JP 1999-535172	19981223
NO 2000003254	A	20000821	NO 2000-3254	20000622
PRIORITY APPLN. INFO.: US 1997-998877 19971224				
WO 1998-US27406 19981223				

AB Novel anti-estrogenic compds., e.g. I [X = hydrocarbyl including at least one O, N, S; X1 = H, hydrocarbyl including at least one O, N, S; X1 = heterocycle; Y = C, N, R1 = H, alkyl, halo, alkylidene; R2, R3 = H, OH, alkyl, alkenyl, aryl, etc.; R4 = H, alkyl; R5 = H, alkoxy, halo, CN, CHO, etc.; R6 = H, alkyl, acyl, aroyl, SO2NH2; R7 = H, halo, NO2, CHO, allyl, amino, etc.; R8 = H, OH, etc.; R9 = H, alkyl; R10 = Me, Et], are prepd. which are useful to treat a variety of disorders, particularly estrogen-dependent disorders. Preferred compds. have 1,3,5-estratriene nucleus, and are substituted at the C-17 or C-11 position with a mol. moiety which renders the compds. effective to competitively block the binding of estrogen to its receptor. Particularly preferred compds. are 17-deoxy-1,3,5-estratrienes. Thus, the citrate salt of II was prepd. and was shown to have antitumor activity against tamoxifen-resistant human mammary carcinoma at a dose of 25mg/kg/day.

MSTR 3

L10 ANSWER 10 OF 16 MARPAT COPYRIGHT 2003 ACS (Continued)



G3 = 23



G4 = 28



G17 = OH
 G24 = Me
 G25 = Ak (SR (1-) G26)
 G27 = O
 G31 = alkyl<(1-24)>
 DER: or pharmaceutically acceptable salts or esters
 DER: or pharmaceutically acceptable salts or esters
 MPL: claim 20
 NTE: oxo substitution also claimed

L10 ANSWER 11 OF 16 MARPAT COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 122:187868 MARPAT
 TITLE: Preparation of .omega.-[4-(dihydroxyestratrien-11.beta.-yl)phenoxy]alkanesulfonamides and analogs as antiestrogens and antiproliferatives
 INVENTOR(S): Nique, Francois; Teutsch, Jean-Georges; Van De Velde, Patrick
 PATENT ASSIGNEE(S): Roussel-UCLAF, Fr.
 SOURCE: Eur. Pat. Appl., 32 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 629635	A1	19941221	EP 1994-401344	19940616
EP 629635	B1	19970319		
FR 2706454	A1	19941223	FR 1993-7310	19930617
FR 2706454	B1	19950515		
HU 67308	A2	19950328	HU 1994-1427	19940506
ZA 9403381	A	19950517	ZA 1994-3381	19940517
US 5494907	A	19960227	US 1994-246190	19940519
JP 07017996	A2	19950120	JP 1994-156407	19940616
CN 1101915	A	19950426	CN 1994-106469	19940616
CN 1054856	B	20000726		
AT 150466	E	19970415	AT 1994-401344	19940616
ES 2099551	T3	19970516	ES 1994-401344	19940616
RU 2140423	C1	19991027	RU 1994-22277	19940616
CA 2126158	AA	19941218	CA 1994-2126158	19940617
AU 9464763	A1	19941222	AU 1994-64763	19940617
AU 673919	B2	19961128		
US 5556845	A	19960917	US 1995-445385	19950519
US 5705494	A	19980106	US 1995-512284	19950808
US 5679788	A	19971021	US 1996-731561	19961016
CN 1271734	A	20001101	CN 1998-108945	19980509
PRIORITY APPLN. INFO.:			FR 1993-7310	19930617
			US 1994-246190	19940519
			US 1995-445385	19950519
			US 1995-512284	19950808

AB Title compds. [I: R = 4-[R1R2NSO2(CH2)n]CGH4; R1, R2 = H, (cyclo)alkyl, acyl, aryl(alkyl), etc.; NR1R2 = heterocyclyl; R3 = H, (cyclo)alkyl, acyl; R17 = OH or acyloxy and R117 = H, alk(en)yl, alkynyl; n .ltoreq. 18] were prepd. Thus, 11.beta.-[4-(4-hydroxyphenyl)estra-4,9-diene-3,17-dione was etherified by CF3CF2CF2CH2NMeSO2(CH2)5I (prepd. given) and the product converted in 3 steps to I [R = 4-[CF3CF2CF2CH2NMeSO2(CH2)5]CGH4, R3 = R17 = H, R17 = OH] which had receptor binding 19, 114, and 55% that of estradiol, dexamethasone, and progesterone, resp., in competitive in vitro assays.

MSTR 1

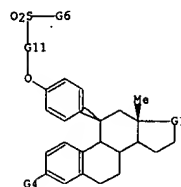
L10 ANSWER 12 OF 16 MARPAT COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 122:81747 MARPAT
 TITLE: Preparation of polyaminosteroids as bactericides and antifungals
 INVENTOR(S): Frye, Leah L.; Zasloff, Michael A.; Kinney, William A.; Moriarty, Robert M.
 PATENT ASSIGNEE(S): Magainin Pharmaceuticals Inc., USA
 SOURCE: PCT Int. Appl., 129 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 5
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9420520	A1	19940915	WO 1994-US2397	19940310
W: AU, CA, JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2157594	AA	19940915	CA 1994-2157594	19940310
AU 9463974	A1	19940926	AU 1994-63974	19940310
AU 692766	B2	19980618		
EP 688333	A1	19951227	EP 1994-911470	19940310
EP 688333	B1	19980819		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 08507527	T2	19960813	JP 1994-520212	19940310
AT 169930	E	19980915	AT 1994-911470	19940310
ES 2123133	T3	19990101	ES 1994-911470	19940310
US 5637691	A	19970610	US 1994-290826	19940818
CA 2185123	AA	19950914	CA 1994-2185123	19940913
WO 9524415	A1	19950914	WO 1994-US10265	19940913
W: AU, CA, JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9480101	A1	19950925	AU 1994-80101	19940913
AU 700344	B2	19981224		
EP 749437	A1	19961227	EP 1994-931274	19940913
EP 749437	B1	20011205		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 09509959	T2	19971007	JP 1994-523429	19940913
AT 210144	E	20011215	AT 1994-931274	19940913
ES 2164110	T3	20020216	ES 1994-931274	19940913
US 5721226	A	19980224	US 1995-478763	19950607
PRIORITY APPLN. INFO.:			US 1993-29018	19930310
			WO 1994-US2397	19940310
			US 1994-290826	19940818
			WO 1994-US10265	19940913
			US 1995-416883	19950420

AB Title compds. [I: X = cationic hydrophilic side chain having .gtoreq.2 pos. charged amino groups; Y = anionic hydrophilic side chain; the steroid nucleus includes satd., unsatd., or partially satd. rings and .gtoreq.1 substituent selected from OH, SH, F, alkyl, alkoxy, amino; with the exception of squalamine) and related compds., were prepd. Thus, 5.alpha.-cholestan-3-one was reductively aminated with BOC-NH(CH2)4N(BOC)(CH2)3NH2 and NaBH3CN in MeOH to give 71% of an .alpha.,.beta.-mixt. of protected cholestan-3-amine which were deprotected with CF3CO2H in CHCl3 to give title compd. II and the .beta.-isomer. II showed a min. inhibitory concn. of 2-4 .mu.g/mL against Staphylococcus aureus, vs. 0.5-1 .mu.g/mL for squalamine.

MSTR 1

L10 ANSWER 11 OF 16 MARPAT COPYRIGHT 2003 ACS (Continued)



G1 = 19



G3 = alkyl<(-8)> (SO (1-) G14)

G4 = OH

G14 = OH / CO2H / alkoxy / carbonyl / CN / acyl / CONH2 /

alkenyl / alkynyl

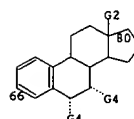
DER: and addition salts

MPL: claim 1

L10 ANSWER 12 OF 16 MARPAT COPYRIGHT 2003 ACS (Continued)



G1 = 66-1 80-3



G2 = alkyl<(1-4)>

G3 = O

G4 = 206



G25 = alkyl<(1-3)>

G26 = alkyl<(1-10)> (SR G27)

G27 = CO2H / OH / CF3

MPL: claim 1

NTE: substitution is restricted

L10 ANSWER 13 OF 16 MARPAT COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 120:31023 MARPAT
 TITLE: Preparation of 11.beta.-thiahydrocarbyl-19-norsteroids and analogs as drugs
 INVENTOR(S): Claussner, Andre; Nique, Francois; Teutsch, Jean
 Georges; Van de Velde, Patrick
 PATENT ASSIGNEE(S): Roussel-UCLAF, Fr.
 SOURCE: PCT Int. Appl., 82 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9313123	A1	19930708	WO 1992-FR1193	19921217
W: AU, CA, FI, HU, JP, KR, NZ, RU, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
FR 2685332	A1	19930625	FR 1991-15856	19911220
FR 2685332	B1	19950602		
IL 104105	A1	19970713	IL 1992-104105	19921215
AU 9333570	A1	19930728	AU 1993-33570	19921217
AU 666916	B2	19960229		
EP 623140	A1	19941109	EP 1993-902339	19921217
EP 623140	B1	19980422		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
HU 68068	A2	19950529	HU 1994-2134	19921217
HU 221482	B	20021028		
AT 165365	E	19900515	AT 1993-902339	19921217
RU 2111213	C1	19980520	RU 1994-31162	19921217
ES 2115754	T3	19980701	ES 1993-902339	19921217
ZA 9209859	A	19931220	ZA 1992-9859	19921218
CN 1075722	A	19930901	CN 1992-115248	19921219
CN 1036718	B	19971217		
US 6281204	B1	20010828	US 1994-244735	19940609
FI 9402944	A	19940617	FI 1994-2944	19940617
US 2002072624	A1	20020613	US 2001-891433	20010626
			FR 1991-15856	19911220
			WO 1992-FR1193	19921217
			US 1994-244735	19940609

AB Title compds. [I: R = XYSOmZ; R3 = H, (cyclo)alkyl, acyl; R7 = H, alkyl, alkenyl, alkynyl, etc.; R16 = H, halo, alkyl; R17 = OH, CH2OH, acyloxy; R7R17 = O, NOH, NNH2, CH2; X = CH2, arylene(oxy); Y = (O-interrupted) (satd.) divalent C1-18 aliph. group; Z = (ar)alkyl, aryl; m = 0-2] were prepd. as antiestrogens, antiproliferatives, etc. Thus, 11.beta.-(4-hydroxyphenyl)estra-4,9-diene-3,17-dione was condensed with Cl(CH2)5Br and the product converted in 3 steps to estratrienediol II [R = C6H4[O(CH2)5Cl]-4] which was condensed with 2-pyridylmethanethiol to give, after oxidn., II [R = C6H4[O(CH2)5SO2]-4, Z = 2-pyridylmethyl]. The latter had relative binding affinity (definition given) of 21.2 at mouse estrogen receptors in vitro.

MSTR 1

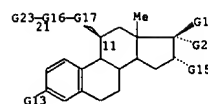
L10 ANSWER 14 OF 16 MARPAT COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 116:214774 MARPAT
 TITLE: 19-Norsteroids having an amide-bearing chain in the 11-beta position, their preparation, their use as medicines (especially antiestrogens), and pharmaceutical compositions thereof
 INVENTOR(S): Claussner, Andre; Nique, Francois; Teutsch, Jean
 Georges; Van de Velde, Patrick
 PATENT ASSIGNEE(S): Roussel-UCLAF, Fr.
 SOURCE: Eur. Pat. Appl., 63 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 471612	A2	19920219	EP 1991-402214	19910809
EP 471612	A3	19920513		
EP 471612	B1	19980128		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
FR 2665901	A2	19920221	FR 1990-10323	19900814
FR 2665901	B2	19940729		
AT 162797	E	19980215	AT 1991-402214	19910809
ES 2112268	T3	19980401	ES 1991-402214	19910809
CA 2049102	AA	19920215	CA 1991-2049102	19910813
HU 59416	A2	19920528	HU 1991-2690	19910813
JP 06340688	A2	19941213	JP 1991-226410	19910813
JP 3073803	B2	20000807		
AU 9182422	A1	19920220	AU 1991-82422	19910814
AU 644671	B2	19931216		
ZA 9106420	A	19921028	ZA 1991-6420	19910814
US 5707982	A	19980113	US 1993-68735	19930528
			FR 1990-10323	19900814
			FR 1989-2384	19890224
			US 1990-484424	19900223
			US 1991-745289	19910814

AB Twenty title steroids I [either (1) n = 1; K = O; R17 = OH, O2C(CH2)2CO2H or salts; R17' = H, C.tpbond.CH; RA = Me; RB = iso-Pr, Bu, heptafluorobutyl; X = CH2, C6H4, OC6H4; Y = (CH2)7, (CH2)8, (CH2)5C.tpbond.C, (CH2)qOCH2 with q = 5-7, (CH2)55(O)pCH2 with p = 0-2; Z = bonds; or (2) n = 1 or 2; K = O, S; R17 = OH, acyloxy; R17' = H, (substituted) alkyl, alkenyl, or alkynyl; or R17R17' = keto; X = CH2, arylene, OCH2, oxyarylene, thiarylene (bound to steroid at C atom); Y = aliph. chain optionally unsatd. or interrupted by arylene, O, S, SO, or SO2; Z = bonds; RA, RB = H, (substituted) alkyl; or RARB = atoms to form (substituted) heterocycle; addnl. restrictions] were prepd. as antiestrogens for treatment of hormone-dependent tumors. For example, 11.beta.-(4-hydroxyphenyl)estra-4,9-diene-3,17-dione was etherified with BuNMCOCH2O(CH2)5Br (prepn. given), followed by isomerization to a 3-hydroxyestra-1,3,5(10)-triene, redn. of the 17-oxo group to 17.beta.-OH with NaBH4, protection of the OH groups as acetates, conversion of the amide to a thioamide with Lawesson's reagent, and deprotection, to give title compd. II. The IC50 of II for inhibiting growth of MCF-7 mammary tumor cells in vitro was 0.03 nM. A tablet formulation comprising I is given.

MSTR 18

L10 ANSWER 13 OF 16 MARPAT COPYRIGHT 2003 ACS (Continued)

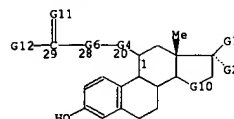


G2 = alkyl(-8) > (SO (1-)) G4)
 G4 = OH / 30 / alkyl(-1-8) > (SO (1-)) X / CN / acyl / alkenyl(-4) > / alkynyl(-4) > / SO / 52

30(O)G6 50(O)G8 52(O)G9

G8 = alkyl (SO OH)
 G13 = OH
 DER: and addition salts
 MPL: claim 1

L10 ANSWER 14 OF 16 MARPAT COPYRIGHT 2003 ACS (Continued)



G2 = alkyl(-8) > (SO (1-)) G3)
 G3 = OH / acyl / COPH / CO2H / alkoxyacetyl / CN / CF3
 G10 = (1-2) CH2
 DER: or salts
 MPL: claim 1
 NTE: substitution is restricted

L10 ANSWER 15 OF 16 MARPAT COPYRIGHT 2003 ACS

ACCESSION NUMBER:

114:43309 MARPAT

TITLE:

Preparation of sulfonic acid-substituted aromatic steroids as inhibitors of steroid 5.alpha.-reductase
Holt, Dennis Alan; Metcalf, Brian Walter; Levy, Mark Alan

INVENTOR(S):

PATENT ASSIGNEE(S):

SmithKline Beecham Corp., USA

SOURCE:

Eur. Pat. Appl., 26 pp.

CODEN: EPOXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 375347	A1	19900627	EP 1989-313260	19891219
EP 375347	B1	19941221		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 4970205	A	19901113	US 1988-290020	19881223
IL 91968	A1	19941021	IL 1989-91968	19891012
CN 1051181	A	19910508	CN 1989-108217	19891024
CA 2005215	AA	19900623	CA 1989-2005215	19891212
ZA 8909669	A	19901128	ZA 1989-9669	19891218
DK 8906451	A	19900624	DK 1989-6451	19891219
ES 2066003	T3	19950301	ES 1989-313260	19891219
AU 8947005	A1	19900628	AU 1989-47005	19891220
AU 627528	B2	19920827		
JP 0225494	A2	19900907	JP 1989-330927	19891220
AU 9229602	A1	19930121	AU 1992-29602	19921214
AU 655691	B2	19950105		

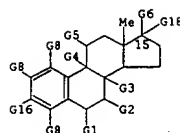
PRIORITY APPLN. INFO.:

AB Title steroids I [X1, X2, X3 = H, Cl, F, Br, iodo, CF3, alkyl, OH, alkoxy, CN, NO2, N(R1)2, CO2R1, CHO; R = (1) .alpha.-H, .alpha.-OH, or .alpha.-OAc, and/or various carbonyl-contg. mono- or divalent radicals, (2) .beta.-acylamino, .beta.-cyano, or .beta.-tetrazolyl and .alpha.-H, (3) keto, etc.; R1 = H, alkyl] and their salts were prepd. For example, Me estrone underwent a sequence of conversion to its enol triflate, aminocarbonylation using (iso-Pr)2NH, hydrogenation of .delta.LTA.16, and demethylation of 3-OMe to give 3-hydroxyestr-1,3,5(10)-triene-17.beta.-(N,N-diisopropylcarboxamide). Acylation of 3-OH with Me2NC(S)Cl, isomerization, and hydrolysis gave the 3-thiol, which was oxidized by O and KOH in DMF to give K estratrienesulfonate deriv. II. The inhibition const. (Ki) of II for steroid 5.alpha.-reductase from hyperplastic human prostate was 10 nM. Ten I are claimed, and preps. with data are given for addnl. precursors of I.

MSTR 2A

L10 ANSWER 15 OF 16 MARPAT COPYRIGHT 2003 ACS

(Continued)



G6 = 36

G7-C(O)-G10

G7 = alkylene<(1-12)>

G10 = alkyl<(1-8)> (SO (1-) OH)

G16 = OH

MPL: claim 8

NTE: also incorporates structure from claim 10

NTE: substitution is restricted

L10 ANSWER 16 OF 16 MARPAT COPYRIGHT 2003 ACS

ACCESSION NUMBER:

112:198890 MARPAT

TITLE:

Preparation of estratriene derivatives as steroid 5.alpha.-reductase inhibitors
Holt, Dennis Alan; Levy, Mark Alan; Metcalf, Brian Walter

INVENTOR(S):

PATENT ASSIGNEE(S):

SmithKline Beckman Corp., USA

SOURCE:

Eur. Pat. Appl., 29 pp.

CODEN: EPOXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

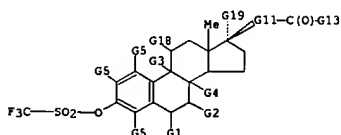
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 343954	A2	19891129	EP 1989-305246	19890524
EP 343954	A3	19900516		
EP 343954	B1	19941130		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
WO 8911282	A1	19891130	WO 1989-US2269	19890523
W: AU, DK, JP				
AU 8937487	A1	19891212	AU 1989-37487	19890523
AU 627466	B2	19920827		
JP 03504498	T2	19911003	JP 1989-506391	19890523
CA 1331457	A1	19940816	CA 1989-600335	19890523
ES 2065378	T3	19950216	ES 1989-305246	19890524
ZA 8903971	A	19900530	ZA 1989-3971	19890525
US 954446	A	19900904	US 1989-380226	19890714
IL 105198	A1	19940227	IL 1989-105198	19891012
DK 9002797	A	19901123	DK 1990-2797	19901123
DK 168295	B1	19940307		
DK 9301303	A	19931119	DK 1993-1303	19931119
DK 169787	B1	19950227		

PRIORITY APPLN. INFO.:

AB The title compds. (I; X1, X2, X3 = H, halo, CF3, Cl-6 alkyl, OH, etc.; A = O, S; n = 0, 1; R1 = H, Cl-8 alkyl; R3 = mono- or divalent radical, e.g., H, alkyl, etc.) (II) useful as steroid 5.alpha.-reductase inhibitors, were prepd. E.g., 17.beta.-(diisopropylcarbamoyl) estr-1,3,5(10)-triene-3-carboxylic acid(II) was prepd. in many steps from estrone via trifluoromethylsulfonylation, carbamoylation, methoxycarbonylation, and hydrogenation. II in vitro inhibited human steroid 5.alpha.-reductase with a Ki of 19 nM. Tablets were formulated contg. I.

MSTR 2F



G11 = alkylene<(1-12)>

L10 ANSWER 16 OF 16 MARPAT COPYRIGHT 2003 ACS

(Continued)

G7 = alkylene<(1-12)>

G13 = alkyl<(1-8)> (SO (1-) OH)

MPL: claim 15

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FILE 'REGISTRY' ENTERED AT 12:20:52 ON 03 APR 2003

L1 STRUCTURE UPLOADED

L2 6 S L1

L3 74 S L1 FULL

FILE 'CAPLUS' ENTERED AT 12:21:43 ON 03 APR 2003

L4 6 S L3

FILE 'REGISTRY' ENTERED AT 12:25:15 ON 03 APR 2003

FILE 'CAPLUS' ENTERED AT 12:26:14 ON 03 APR 2003

L5 6 S L3

L6 0 S L5 NOT L4

FILE 'BEILSTEIN' ENTERED AT 12:26:28 ON 03 APR 2003

L7 7 S L1 FULL

FILE 'USPATFULL' ENTERED AT 12:29:26 ON 03 APR 2003

L8 0 S L3

FILE 'MARPAT' ENTERED AT 12:29:56 ON 03 APR 2003

L9 17 S L3 FULL

L10 16 S L9/COM